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Volume 2. Systems Manual

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16. ABSTRACT

This report describes the Systems Applications, Inc. (SAI) Airshed Model System from a programmer's point of view. Included are discussions of all subroutines and how they fit together, run-time core allocation techniques, internal methods of segment handling using secondary storage, and detailed definitions of the structure of each file in the system. This manual also includes suggestions for implementing the programs on different computers.

The SAI Airshed Model System consists of 17 programs that communicate with each other through 17 data files; both the programs and files are described in detail in this manual. Chapter II presents an overview of the system, briefly describing the programs used to perform each of the five system functions.
Chapter III contains guidelines for implementing the programs, and Chapters IV through VIII contain detailed descriptions of the programs by function, including hierarchical subroutine tables and short module descriptions. Chapter IX contains detailed file structure definitions for each file in the system.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

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ABBREVIATIONS

act	activation
add	additive
b	boundary
bd	bound
beg	beginning
B.T.	Boundary Table
chem	chemistry
coeff	coefficient
col	column
conc	concentration
const	constant
crit	criterion
dark	darkness
diam	diameter
fact	factor
ht	height
i	initial
iter	iteration
LBL	Lawrence Berkeley Laboratory
loc	location
low	lower
L.T.	Local Table
max	maximum
M.E.B.	meteorology, emissions, and initial and boundary conditions
meth	method
min	minimum
molec	molecular
mult	multiplicative
num	numerical
param	parameter

pr	print
prof	profile
pt	point
srce	source
reac	reaction
ref	reference
rel	relative
resis	resistance
spec	species
S.S.T.	Segment Scratch Table
S.T.	Segment Table
stn	station
st-st	steady-state
subreg	subregion
surf	surface
temp	temperature
tol	tolerance
u-def	user-defined
up	upper
UTM	Universal Transverse Mercator
val	value
var	variable
vartn	variation
vel	velocity
vert	vertical
wt	weight

I INTRODUCTION

This report presents a general view of the Systems Applications, Inc. (SAI) Airshed Model as well as detailed operating instructions for the user. Included are discussions of all the files needed to run the model, the data preparation programs that produce each file, the input formats and data preparation methods, samples of input and output, and information flow diagrams that illustrate the job stream control on any computer.

Chapter II presents a technical summary of the SAI Airshed Model; Chapter III contains an overview of the model as a system of computer programs, outlining the five main functions that must be performed by users and programs together. Chapter IV discusses some of the concepts and terms basic to an understanding of the system, followed in Chapter V by descriptions of the job control notations that will be used throughout this manual. Chapters VI through XI examine in detail the five main functions of the system, providing input and output definitions and examples, and job control diagrams for each program that must be exercised.

The Systems Manual, the companion to the User's Manual, describes the system from a programmer's point of view. Included are descriptions of all subroutines and how they fit together, run-time core allocation techniques, internal methods of segment handling using secondary storage, and detailed structure definitions of all files in the system. The Systems Manual also discusses procedures for implementing the programs on different computers, and the addition, removal, or replacement of computing algorithms and data preparation methods.

II THE SAI AIRSHED MODEL

Systems Applications, Incorporated (SAI) designed its Airshed Model to calculate the concentrations of both reactive and inert air pollutants through simulation of the numerous physical and chemical processes that take place in the atmosphere. Much of the current interest in the model arises from the need to calculate ozone concentrations as a part of various environmental assessment studies (such as federally required State Implementation Plans and New Source Reviews). The results of recent evaluation and applications studies indicate that the SAI Airshed Model provides a sound, practical, and effective means for analyzing a variety of regional air quality problems.

Interactions among organic compounds (including pure and oxygenated hydrocarbons and other hydrocarbon derivatives) and nitrogen oxides (NO_x) are usually responsible for the relatively high ozone concentrations observed in and downwind of urban areas. Among the main factors affecting photochemical air quality in urban areas are:

- The spatial and temporal distribution of emissions of NO_x and organic species.
- The composition of the emitted organic species.
- The spatial and temporal variations of the wind field.
- The stability of the atmosphere and the associated dynamics of the mixing layer.
- The chemical reactions involving organic species and NO_x.
- The diurnal variations of ultraviolet radiation.
- The loss of ozone and its precursors by surface uptake processes.
- The ambient background concentrations of ozone, organic species, and NO_x immediately upwind of the urban area and within an elevated inversion layer.

Thus, development of an accurate ozone prediction relationship requires investigation of the relevant physical and chemical atmospheric phenomena that influence the magnitude and distribution of both ozone and its precursors.

To limit ozone concentrations, one must control all or part of the ozone formation process. Practically, man has the most influence on anthropogenic emissions. If ozone concentrations were proportional to emissions of organic compounds or NO_x, it would be simple to calculate the reduction in anthropogenic emissions necessary to achieve a desired reduction in ozone concentrations. But the relationship between ozone air quality and emissions of NO_x or organic species is complicated and nonlinear. Furthermore, the relationship changes with location and even with time at a given location because of variations in emissions, meteorology, and other factors.

To make available an appropriate quantitative treatment of this relationship, the U.S. Environmental Protection Agency (EPA) has, through a multiyear research effort, supported the development of the SAI Airshed Model. Initial model development efforts and applications (to the Los Angeles area) are fully described in a 15-volume series of reports by Roth et al. (1971) and Reynolds et al. (1973a). These reports are summarized in the three papers by Reynolds et al. (1973b, 1974) and Roth et al. (1974). Evaluation of the model's predictions and its components at that time showed that improved treatments of some physical and chemical processes were necessary. As a result, another series of research efforts was carried out to improve the model. These efforts are described in a 7-volume series of reports by Jerskey and Seinfeld (1976), Jerskey et al. (1976), Killus et al. (1977), Lamb (1976), Lamb et al. (1977), Liu et al. (1976a), and Reynolds et al. (1976), and in the papers by Lamb et al. (1975), Liu and Seinfeld (1975), Liu et al. (1976b), and Reynolds (1977). A summary of the technical features included in this model is given in the report by Reynolds et al. (1982).

A. THE TECHNICAL FEATURES OF THE SAI AIRSHED MODEL

The SAI Airshed Model can simulate the dynamic behavior of up to 20 pollutants. When photochemical simulations are carried out, 11 species must be included: nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), single-bonded carbon atoms (PAR), double-bonded carbon atoms except ethylenes (OLE), aromatic-bonded carbon atoms (ARO), carbonyl-bonded carbon atoms, ethylene, benzaldehyde (BZA), peroxyacetyl nitrate (PAN), and carbon monoxide (CO). In addition, the model can provide predictions of SO_2 and aerosol.* The user can exercise any of the following options with respect to the pollutants to be simulated:

> Up to 20 unreactive pollutants.
> Photochemical species, CO,[†] and up to 9 other unreactive pollutants.
> Photochemical species, CO, SO_2, and up to 8 other unreactive pollutants.
> Photochemical species, CO, SO_2, aerosol,[§] and up to 7 other unreactive pollutants.
> Photochemical species, CO, aerosol,** and up to 8 other unreactive pollutants.

As illustrated in Figure II-1, simulations are performed on a three-dimensional grid selected by the user to cover the region of interest. Figure II-1 also shows the various atmospheric processes treated in each grid cell. The base of an elevated inversion layer is often selected as the top of the grid, but the model includes provisions to facilitate treatment of the inversion layer itself. The model's computer codes can handle any number of cells in the horizontal and vertical directions.

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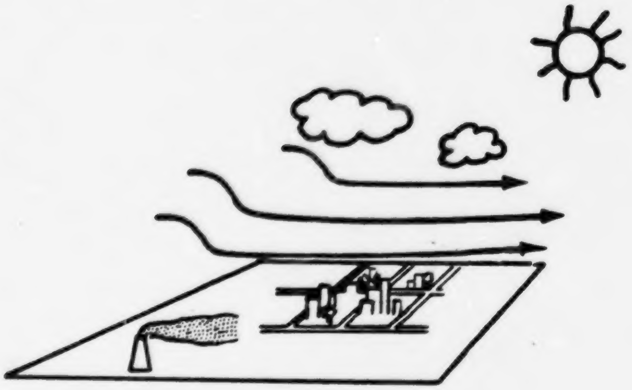
* The aerosol component includes emitted particulates and organic, nitrate, and sulfate aerosols formed in the atmosphere.

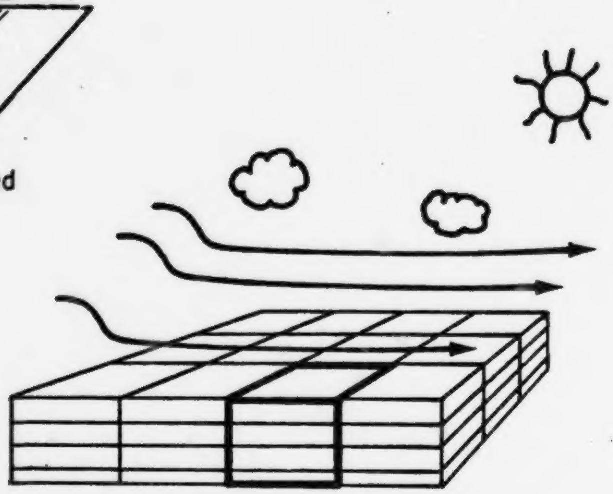
[†] Photochemical species include the first 10 pollutants cited above.

[§] This aerosol consists of organic, nitrate, and sulfate components.

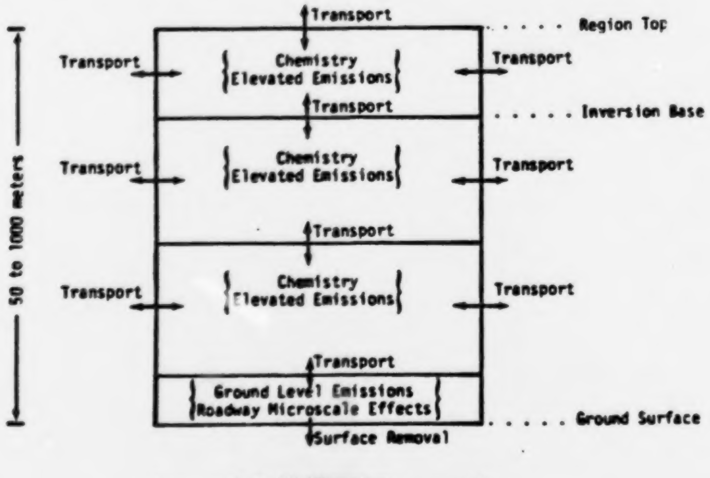
** This aerosol consists of only the organic and nitrate components.



(a) The Area To be Modeled



(b) Specification of the Grid


Transport
Region Top
Transport
Chemistry
Elevated Emissions
Transport
Transport
Inversion Base
Transport
Chemistry
Elevated Emissions
Transport
Transport
Transport
Chemistry
Elevated Emissions
Transport
Transport
Ground Level Emissions
Roadway Microscale Effects
Ground Surface
Surface Removal
50 to 1000 meters
1 to 10 Kilometers

(c) Atmospheric Processes Treated in a Column of Grid Cells

Figure II-1. Schematic Illustration of the Grid Used and Treatment of Atmospheric Processes in the SAI Airshed Model

1. Treatment of Atmospheric Chemistry

Ozone is not emitted from sources; rather, it is formed by chemical reactions in the atmosphere. Consequently, to calculate ozone concentrations, a physicochemical model must contain a kinetic mechanism, that is, a group of chemical reactions and rate constants intended to represent the ozone formation process. Because of computing time limitations, it is not possible to include explicitly each chemical species of interest; thus, most of these kinetic mechanisms treat organic compounds in groups, often on the basis of the reactive functional groups they contain. For example, propylene, 1-butene, and 1-pentene, which each contain a carbon-carbon double bond, can be aggregated together as a single "lumped" species. Such a mechanism was used in the airshed model until 1976, when the Carbon-Bond Mechanism was developed.

Because of the association of reactions and reactivities with carbon bonds, the range of reactions and rate constants to be treated in a kinetic mechanism can be narrowed considerably when each carbon atom is treated according to its bond type. This concept is the basis for the Carbon-Bond II Mechanism, a 65-reaction mechanism developed at SAI and employed in the SAI Airshed Model (Whitten and Hogo, 1977; Whitten, Killus and Hogo, 1980). In this mechanism, the carbon atoms of each organic compound are assigned to one of the following groups: single-bonded carbon atoms, double-bonded carbon atoms except ethylene, ethylene, aromatic-bonded carbon atoms, carbonyl-bonded carbon atoms, and benzaldehyde. Further discussion of the definition and treatment of these groups is given in the final report on the application of the model to the Tulsa urban area (Reynolds et al., 1982). The user can add to the mechanism four reactions describing SO_2 oxidation and reaction expressions accounting for the formation of sulfate, organic, and nitrate aerosol products.* Simulations of smog chamber experiments indicate that the Carbon-Bond Mechanism performs significantly better than those previously employed in the airshed model (Whitten, Hogo, and Killus, 1980).

---

* The 69-reaction mechanism is shown in Chapter IX and is discussed in more detail in Reynolds et al. (1982).

2. Treatment of Advective Pollutant Transport

Pollutants are transported primarily by advection, that is, by the mean or bulk motion of the wind. A major difficulty in treating advection is wind shear, the variation of the wind with altitude. The wind speed near the ground typically increases with height, but the wind several hundred meters aloft may be faster or slower--and frequently from a different direction. In the original airshed model, wind shear was neglected, but later sensitivity studies indicated that inclusion of wind shear effects in the model could significantly alter NO_2 and ozone predictions (Reynolds et al., 1976). Consequently, the capabilities of the model were expanded to treat wind shear phenomena. Theoretical wind shear relationships were derived by Lamb (1976) using the predictions of a planetary boundary layer model developed by Deardorff (1972). These relationships are useful when wind measurements aloft are not available. When wind measurements are available both at the surface and aloft, one or more objective techniques are used to prepare appropriate three-dimensional wind inputs to the model. Two algorithms in the model are described by Liu et al. (1973) and Killus et al. (1977).

3. Treatment of Turbulent Diffusion

Pollutants are transported and dispersed largely by the action of the wind rather than by molecular diffusion. The treatment of advection discussed above does not represent pollutant transport completely because it ignores the influence of small-scale features of the wind, called eddies. Describing these microscale features of the wind deterministically is difficult because available data are insufficient to characterize winds on such a fine scale. Consequently, it is necessary to parameterize the microscale turbulent diffusion processes. In the SAI Airshed Model, and most other grid models as well, transport of a pollutant by turbulent diffusion is assumed to be proportional to the rate of change of concentration with position (i.e., concentration gradient). The proportionality factor is termed the eddy diffusivity coefficient. These coefficients are sometimes treated as constants, but they can more accurately be treated as functions of atmospheric stability, surface roughness, and height above the ground.

Because of the empirical nature of the eddy diffusivity concept, it has heretofore been difficult to obtain precise measured or theoretical estimates for the diffusivity coefficients. At SAI, considerable effort has been devoted to the study of turbulent transport processes. As a result of these efforts, we have developed a novel procedure for estimating diffusivity coefficients. In this approach, control theory techniques are employed in conjunction with the results of a sophisticated planetary boundary layer model to generate "optimal" diffusivity values. For further details, the reader is referred to the reports by Lamb (1976) and Lamb et al. (1977).

4. Treatment of Other Microscale Phenomena

Several phenomena besides turbulent diffusion have characteristic spatial or temporal scales too small for explicit, deterministic resolution in urban and regional grid models. Two important examples are the rise of a hot, buoyant emissions plume from a large point source and the scavenging of ozone near roadways by NO emitted from vehicles. Studies of these phenomena and others at SAI resulted in the incorporation of an improved treatment of plume rise from point sources. In addition, a preliminary version of a module to treat the microscale effects of the emissions from a network of line sources (e.g., highways) in the lowest layer of grid cells has also been developed. In this layer, taken to be about 20 meters deep, NO emissions from vehicles on a roadway are allowed to react only with the ozone in the immediate vicinity of the roadway. More detailed descriptions of these algorithms and other microscale phenomena are given by Lamb (1976) and Lamb et al. (1977). Since the performance of the microscale module has not been thoroughly evaluated, we do not recommend that this optional model feature be exercised at this time.

5. Treatment of Surface Removal Processes

Many types of pollutants, including NO_2, ozone, and SO_2 in particular, can be removed from the atmosphere by chemical reaction, adsorption, or absorption at various surfaces found in urban areas. A methodology for calculating the removal of gaseous pollutants by surface sinks has been incorporated in the model. Surface removal is assumed to take place in two steps: transport to the surface followed by uptake by the surface. Parameterization of this two-step process is accomplished by defining a resistance to mass transport and a resistance to surface removal. The transport resistance is estimated from theoretical considerations of turbulent transfer in the atmospheric boundary layer, and the surface resistance is obtained from experimental data on the uptake of pollutants by various types of surfaces (Killus et al., 1977).

6. Other Technical Features

The numerical procedure used to solve the conservation-of-mass equations for each pollutant is an important component of a grid model. To minimize the propagation of numerical errors, techniques for treating horizontal (advective) pollutant transport--an element of the model particularly difficult to handle numerically--were examined. The results of these studies indicated that, of the techniques examined, the SHASTA integration scheme provided the best balance between accuracy of prediction and computational speed (Reynolds et al., 1976; Killus et al., 1977).

The SAI Airshed Model contains features designed to reduce cost by minimizing labor and computing expenses. For example, computerized data preparation programs are available for automating the conversion of various types of data into the proper input format. These features have no effect on the model's treatment of atmospheric processes, but they do aid the user in preparing the inputs required by the Airshed Model.

The model output consists of the predicted pollutant concentrations for every grid cell. These predictions are generally averaged over a period of one hour and are saved on a computer file for subsequent display and analysis. An example of the printed output produced by the display program is given in Figure II-2. If other computer graphics capabilities are available, then the results can be plotted as shown in Figures II-3 and II-4. Note, however, that the computer programs described in this manual produce only printed displays of the predicted concentrations. Gridded census data can be used in conjunction with the model predictions to estimate the dosages and exposures that are experienced by the human population within the modeling region. The results of an exposure analysis carried out for Denver are shown in Figure II-5. Of course, other displays and analyses can be prepared depending on the needs of the user.

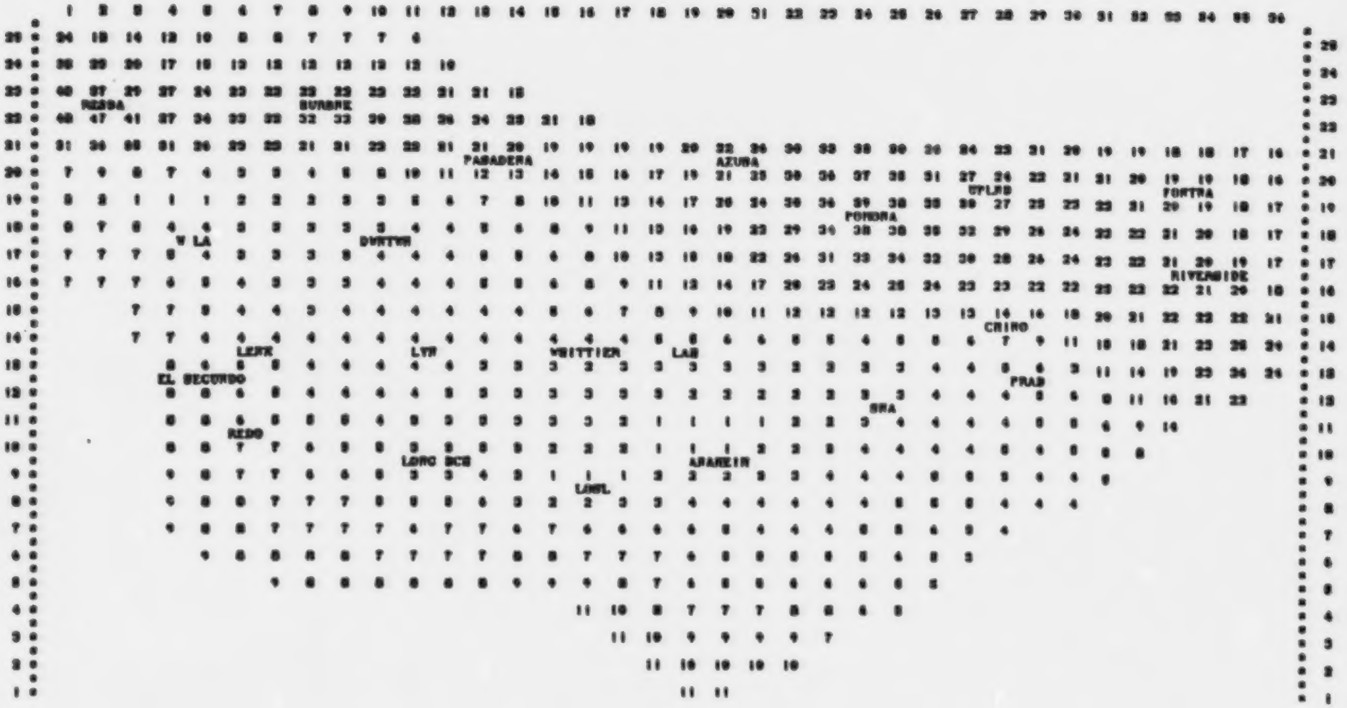
B. MODEL USAGE

In general, studies that employ the SAI Airshed Model can be segmented into three phases: adaptation, evaluation of validity and performance, and application. The specifics of each phase depend on the region to be modeled and the intended application, but certain characteristics apply to each case.

The primary objective of Phase I is to adapt the model for application to a particular region. Efforts involved in this undertaking include:

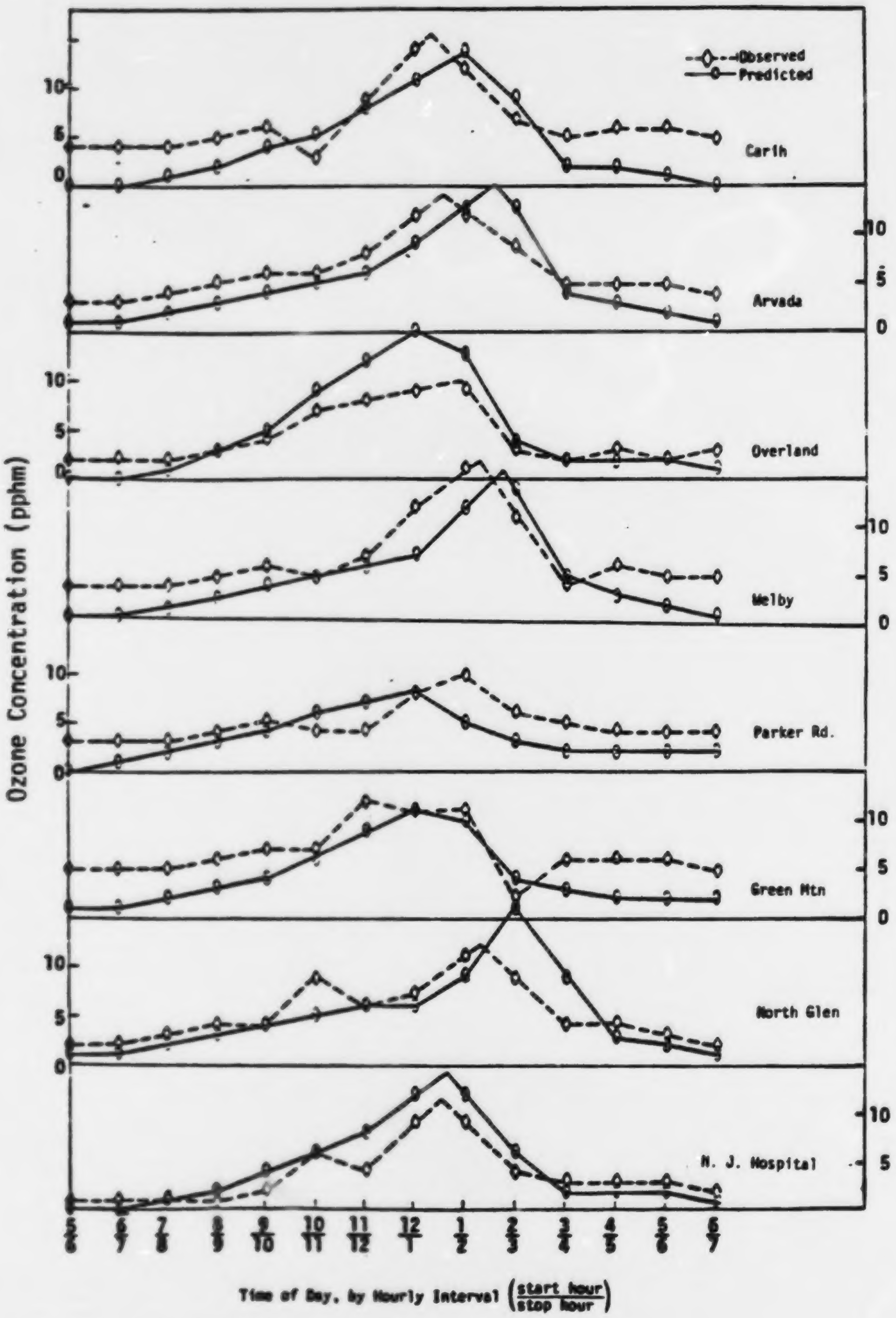
> Review of pertinent air quality studies of the region.
> Examination and assessment of available emissions and aerometric data.
> Specification of supplemental data (if any) needed for verification and application of the model.
> Collection of supplemental data, if necessary, through intensive field monitoring studies.
> Adaptation of existing, or development of new, input data preparation programs.

Upon completion of these tasks, the user is in a position to carry out photochemical simulations with the model.


RESDA
BURBNK
PASADENA
AZUSA
UPLND
FONTNA
POMONA
W LA
DWNTWN
RIVERSIDE
CRINO
LENX
LYN
WHITTIER
LAH
PRAD
EL SECUNDO
SNA
REDO
LONG BCH
ANAHEIM
LNHL

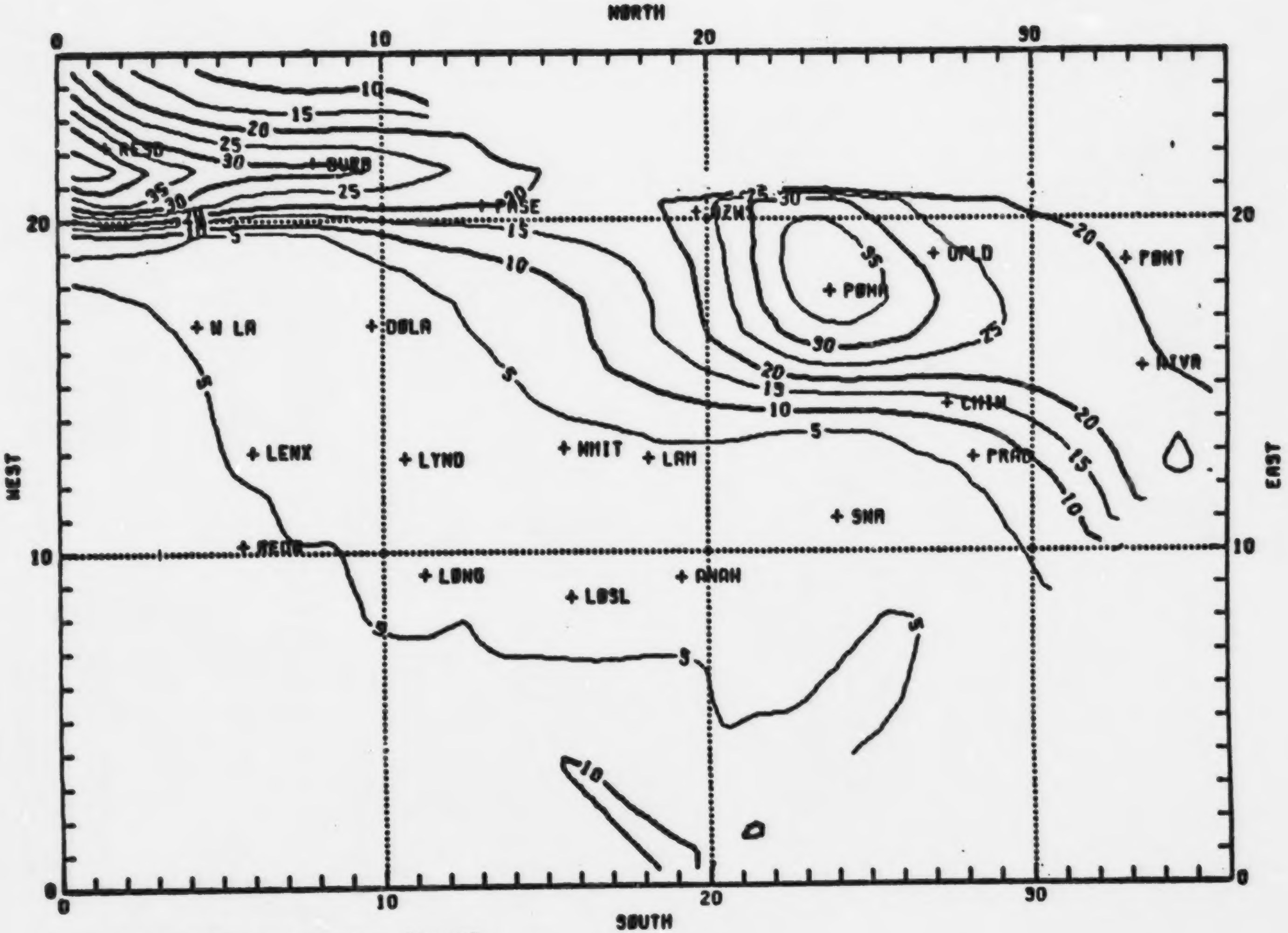
Source: Tesche and Burton (1978).

Figure II-2. Example of a Printed Map of Ground-Level Concentration Predictions. Average ground-level O_3 concentrations (pphm) are given for Los Angeles on 4 August 1975 between 1:00 and 2:00 p.m. PST.



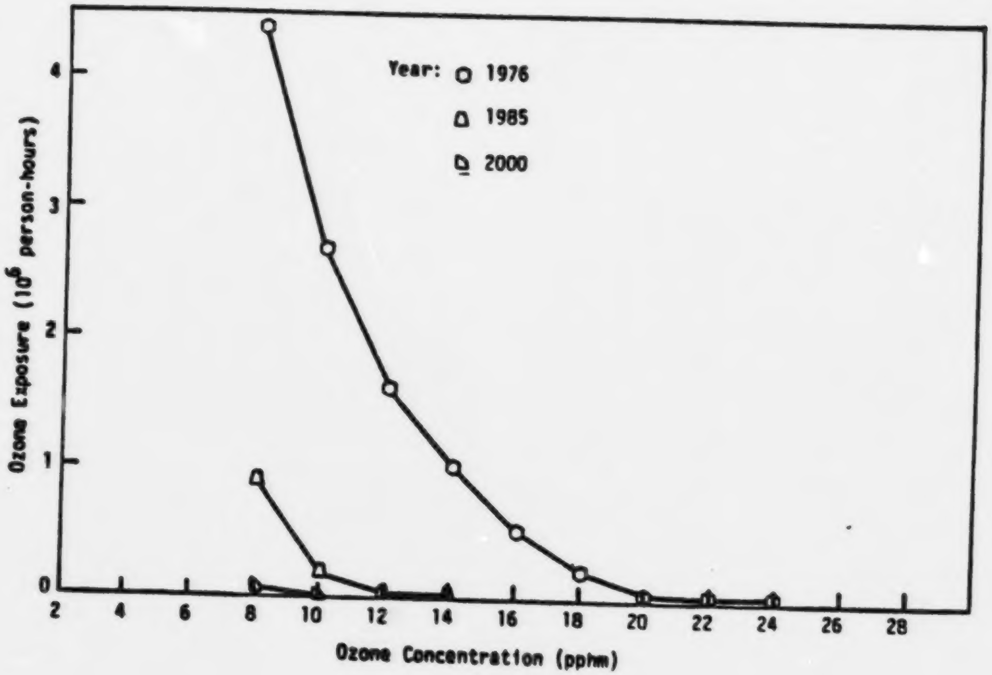
Source: Anderson et al. (1977).

Figure II-3. Example of Plots Illustrating Model Predictions and Actual Measured Concentrations. Ozone concentrations measured at various stations in the Denver area on 28 July 1976 are compared with the corresponding predictions of the SAI Airshed Model as modified for Denver.


NORTH
SOUTH
WEST
EAST
0
10
20
30
+ RESD
+ BURB
+ PASE
+ AZWI
+ POMA
+ UPLD
+ PONT
+ RIVR
+ W LA
+ DOLA
+ LENX
+ LYND
+ WHIT
+ LAH
+ CHIN
+ PRAD
+ SNA
+ REDN
+ LONG
+ LOSL
+ ANAH
5
10
15
20
25
30
35

Source: Tesche and Burton (1978).

Figure II-4. Example of a Plotted Contour Map of Ground-Level Concentration Predictions. Average ground-level O_3 concentrations (pphm) are given for Los Angeles on 4 August 1975 between 1:00 and 2:00 p.m. PST.



Source: Anderson et al. (1977)

Figure II-5. Example of the Results of a Population Exposure Analysis: Denver

Phase II is devoted to assessing the performance of the model. First, the model is used to simulate the formation of photochemical smog on one or more days in the past chosen to represent typical or episodic meteorological conditions. Model predictions are then examined in light of actual observations in an effort to characterize model performance (see Figure II-3). Tasks in this phase include:

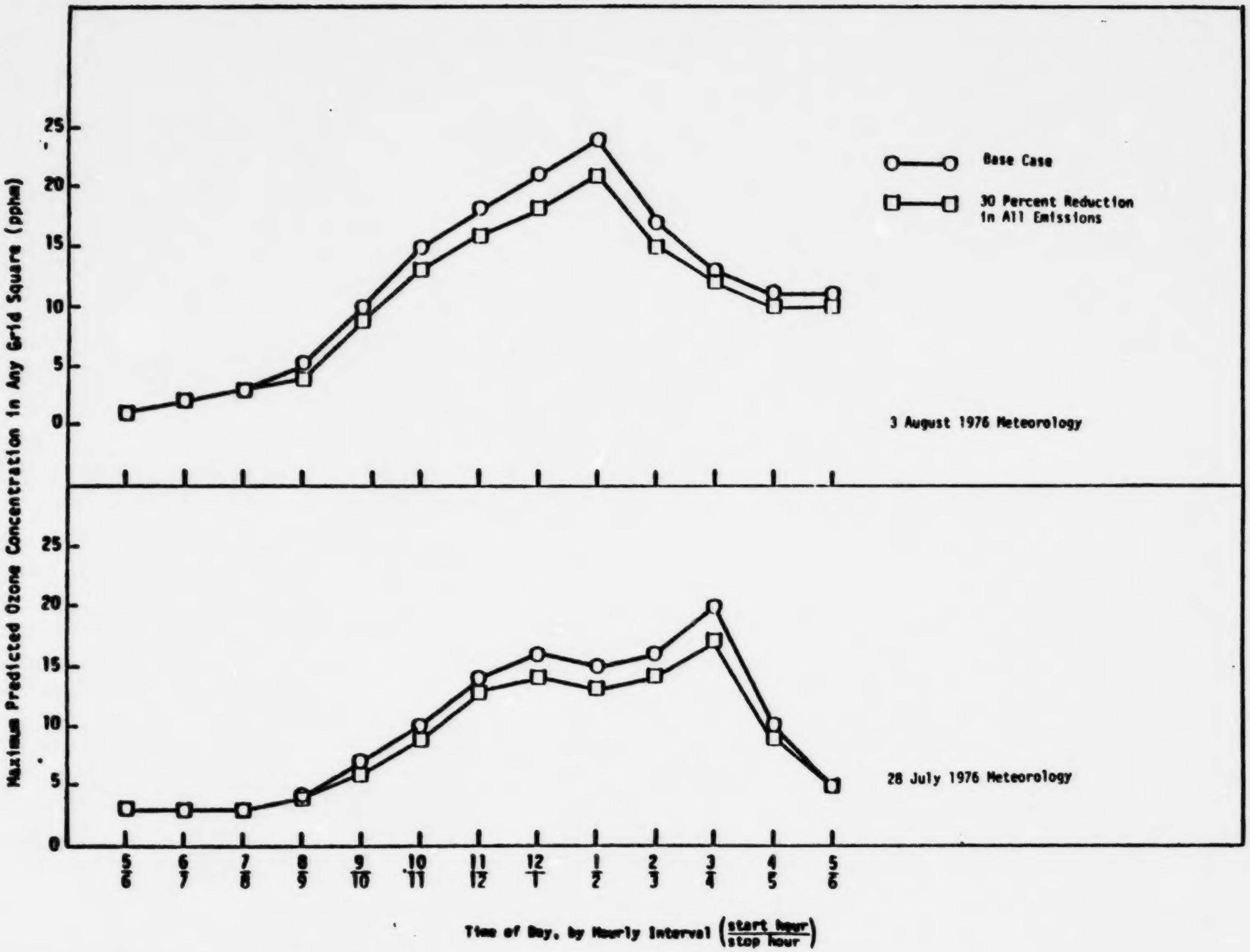
> Selection of days for testing.
> Preparation of model inputs for each day.
> Performance of model simulations and analysis of results.
> Collection of additional data, modification of the model or input data preparation programs, or both, as needed, until satisfactory model performance is obtained.

After the model has been demonstrated to perform adequately, further applications studies can be carried out with reasonable confidence.

The intent of the air quality modeling study is not fully realized until Phase III, when control issues are addressed. Applications of the model generally involve the following tasks:

> Definition of the scenarios to be considered.
> Specification of input conditions for each scenario (for example, adverse meteorological conditions, weekday emissions, and so on).
> Performance of model simulations and analysis of results.

In evaluating the effects of some change in emissions, one compares the predictions for that case with those for a base case (see Figure II-6). The base case might, for example, represent conditions without the imposition of emissions controls. Several measures can be examined in assessing the effects of emissions alterations, including maximum one-hour-average concentrations, population dosages, and area-wide concentration changes. Of course, the model predictions can also be compared



Source: **Anderson et al. (1977).**

Figure II-6. Sample Results of Phase III--Simulation of Emission Control Scenarios. Ozone concentrations predicted by the SAI Airshed Model for the Denver area for 1976 emissions and a 30 percent emissions reduction are shown; note that reducing emissions of both NO_x and organic species by 30 percent reduced the maximum predicted ozone concentration by about 15 percent.

with air quality standards. As shown in Figures II-5 through II-7, various graphical techniques can be employed to display the model results.

C. MODEL APPLICATIONS

Many seemingly straightforward but inherently difficult issues arise in planning for the abatement and control of air pollution in an urban area. Some of these issues can best be addressed through the use of an airshed model; others can be addressed only in this way. This section discusses potential model applications and summarizes studies performed through June 1978 that employed the SAI Airshed Model.

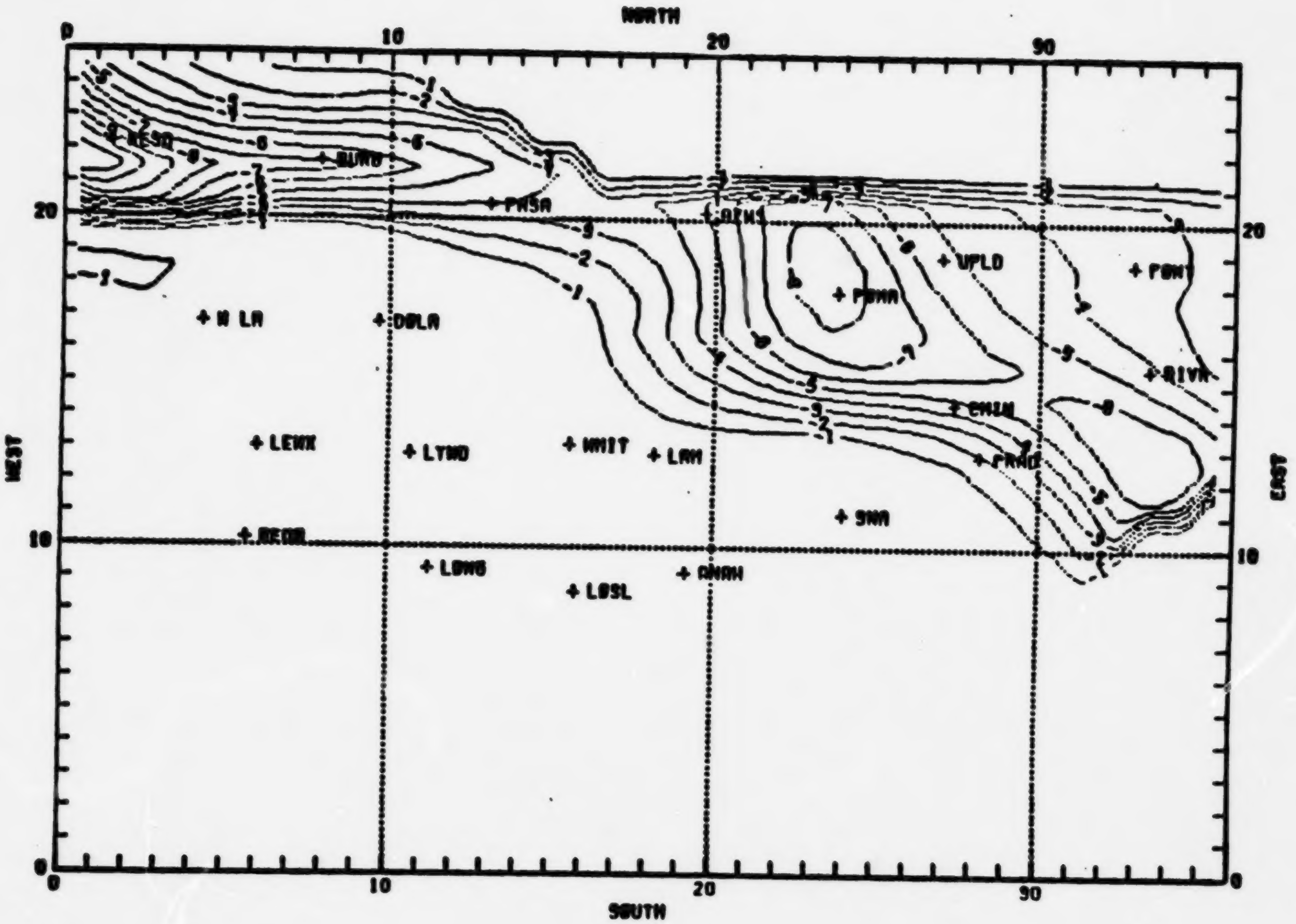
Analyses that can be carried out with the SAI Airshed Model include:

> Development of an emissions control policy. For example, the model can be applied to cities to ascertain the influence of various potential motor vehicle emissions standards on ambient CO, ozone, and NO_2 concentrations.

> Evaluation of proposed emissions control strategies. The model would be particularly useful in helping to establish estimates of the relative emissons reductions of organic species and NO_x required to achieve the ozone and NO_2 air quality standards.

> Selection of sites for future sources of air contaminants. Of particular interest here is the examination of alternative future source development scenarios that would minimize the possibility of subsequent violations of air quality standards.

> Planning for the control of air pollution episodes. The model can be used to ascertain either the extent of intermittent controls required to relieve episodic conditions or the effectiveness of alternative control measures, such as emissions reductions in various portions of a region.


NORTH
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+ BURK
+ PASA
+ AZUS
+ UPLD
+ FONT
+ POMA
+ RIVR
+ CHIN
+ PRAD
+ N LA
+ DOLA
+ LENX
+ LYND
+ WHIT
+ LAH
+ SNA
+ REDB
+ LONG
+ LOSL
+ ANAH

Source: Tesche and Burton (1978).

Figure II-7. Contour Plot Illustrating the Predicted Effect of a Control Strategy. This figure indicates the predicted effect on O_3 levels in the Los Angeles area of a 50 percent reduction in motor vehicle emissions of NO_x and organic species. The O_3 isopleths (pphm) represent the difference between the control strategy and base case predictions for the hours 1:00 to 2:00 p.m. PST.

> Assessment of the contributions responsible for existing levels of air pollution. The model can be exercised both with and without particular sources included in the emissions inputs to examine their contributions to existing air quality.

> Estimation of air quality in areas for which pollutant concentration data are unavailable. Model predictions can be used to locate regions experiencing high pollutant concentrations and thus aid in selecting additional monitoring sites.

In general, applications such as those cited above are carried out by altering any of four inputs to the model: the spatial distribution of emissions, the temporal distribution of emissions, the composition of organic compounds emitted from sources, and the initial and boundary pollutant concentrations. Control strategies that attempt to alter the reactivity of organic species emitted into the air, such as solvent substitution measures, can be handled in the model by altering the magnitude and composition of the emissions from the appropriate sources. In addition, emissions from one city may be responsible for increased background pollutant concentrations in a city downwind. The effects of alterations in background concentrations can be examined through changes in the initial and boundary pollutant concentrations used as input to the model.

Besides these applications, the SAI Airshed Model can be used in other photochemical air pollution analyses. Sensitivity studies, for example, can help assess the relative influences of various physical and chemical processes on pollutant concentrations in a particular region. Such information might be used as a basis for simplifying the treatments of various processes in the model or for reducing the amount of input data to be collected. Moreover, the model can serve as an educational tool by enhancing the existing understanding of the causes of photochemical air pollution in the region. The SAI Airshed Model can also be employed to test new theories, algorithms, and parameterizations of atmospheric processes. Thus, the model is useful in applications ranging from the evaluation of emissions control strategies to the advancement of knowledge in atmosperic science.

Initially, most applications of the SAI Airshed Model were in research projects aimed at improving the model's components or in evaluative studies to ascertain its performance. However, several studies have been carried out that are illustrative of the applications cited earlier. We list below several of these investigations carried out through 1978 that the user can refer to for information on applying the model to suit specific needs.

> An evaluation of four motor vehicle emissions control strategies for Los Angeles. The scenarios included (1) a 30 percent reduction in vehicle mileage, (2) a 100 percent reduction in vehicular emissions, (3) 79 percent, 73 percent, and 62 percent reductions in the emissions of organic species, NO_x and CO, respectively (strategy proposed by the Environmental Quality Laboratory at Caltech), and (4) a 90 percent reduction in vehicle mileage in the downtown Los Angeles area (Reynolds et al., 1973a).

> An examination of a proposed State Implementation Plan for Los Angeles (June 1973). Three scenarios were considered in this study: (1) baseline 1969 conditions, (2) baseline 1977 conditions (with existing legislation in force), and (3) 1977 conditions with additional emission reductions resulting from gasoline rationing, carpooling, implementation of special bus lanes and parking restrictions, and limited control of stationary sources (Reynolds and Seinfeld, 1975).

> An analysis of air quality for the Denver metropolitan region for the years 1976, 1985, and 2000. This study examined the impact on air quality of the urban growth associated with the construction of new wastewater treatment facilities. Model runs were also made to ascertain the sensitivity of the predictions to various land use scenarios that involved alterations to the spatial

distribution of emissions (Anderson et al., 1977). Samples of the results are given in Figures II-3, II-5, and II-6.

> A demonstration of the model's utility in selecting sites for aerometric monitoring. As part of a study sponsored by the EPA Environmental Monitoring and Support Laboratory in Las Vegas, the SAI model was applied to Las Vegas and the predictions were employed to estimate the best locations for CO monitors (Liu et al., 1977).

> An examination of the influence of highway location, design, and operation on photochemical smog formation. This study, sponsored by the Federal Highway Administration, is evaluating various transportation control strategies and will provide guidance to highway personnel in the use of photochemical models (Reynolds et al., 1979).

> An analysis of model sensitivity to ascertain the relationships between the quantity of data collected for use in estimating model inputs and the performance of the SAI Airshed Model. This information will be integrated into a larger study for the EPA Office of Air Quality Planning and Standards (OAQPS) aimed at examining means for employing the SAI model in evaluating the performance of simple oxidant relationships (Tesche et al., 1981).

> An examination of the capability of the SAI model to resolve the impact of emissions from major elevated point sources on regional air quality. Sponsored by the Southern California Edison Company, this study focused on the influence of NO_x and SO_2 emissions reductions on the expected incremental changes in NO_2, ozone, and sulfate levels aloft and at the ground in the Los Angeles area (Tesche and Burton, 1978).

> An evaluation of alternative population growth scenarios for the Los Angeles metropolitan area. The purpose of this study is to help regional planners at the Southern California Association of Governments determine the extent to which future air quality levels in 1990 will be sensitive to the

manner in which the area is allowed to develop over the next 12 years.

Other ongoing studies that are not direct applications of the model but that do have some bearing on model usage include:

> An investigation to establish guidelines for setting model performance measures and standards. This study for the OAQPS will yield information that will aid in evaluating the suitability of a model for use in a particular application (Hayes, 1978).

> A study to establish guidelines for validation of air quality models. This effort will provide guidance to users in the examination of model performance. This study is also being carried out for OAQPS (Hillyer, Reynolds, and Roth, 1979).

In addition to these studies, versions of the SAI Airshed Model have been implemented for use in several cities, both in this country and in Europe. Table II-1 summarizes these applications.

TABLE II-1. USE OF THE SYSTEMS APPLICATIONS (SAI) AIRSHED MODEL IN STUDIES OF AIR QUALITY IN URBAN AREAS.

User	Model Version	Study Site	Sponsor and Reference
Systems Appl., Inc.	1973	Los Angeles	EPA, Contracts CPA 70-148 and 68-02-0339 (Reynolds, 1973)
Systems Appl., Inc./ CAL TRANS/CARB	1973	Los Angeles	California Department of Transportation, Contract K-7319; California Air Resources Board, Contract ARB 4-250
Systems Appl., Inc.	1973	Los Angeles	Texaco
Systems Appl., Inc.	1973	Los Angeles	Western Oil and Gas Association
Systems Appl., Inc.	1977	Los Angeles	DOT, Contract DOT-FH-11-8529 (Reynolds et al., 1979)
Systems Appl., Inc.	1977	Los Angeles	Southern California Edison Company (Tesche and Burton, 1978)
Systems Appl., Inc.	1977	Los Angeles	Southern California Association of Governments (Reynolds et al., 1978)
Systems Appl., Inc.	1978	Los Angeles	Southern California Association of Governments and South Coast Air Quality Management District
Systems Appl., Inc.	1978	Los Angeles	NCAQ Contract (Souten, Tesche, and Oliver, 1981)
Systems Appl., Inc.	1982	Los Angeles	Western Oil and Gas Association (Roth et al., 1984)
Systems Appl., Inc.	1978	Tulsa	EPA Contract 68-02-3370 (Reynolds et al., 1982)
Systems Appl., Inc./ TNO	1978	The Netherlands	TNO (Builtjes et al., 1982)
Systems Appl., Inc./ Freie Universität Berlin/TNO	1978	Bonn/Cologne	Stern and Scherer (1982)
Systems Appl., Inc.	1978	California Central Valley	PG&E
Systems Appl., Inc.	1978	Los Angeles	EPA, Contract 68-02-2870 (Tesche et al., 1981)

Continued

TABLE II-1 (Concluded)

User	Model Version	Study Site	Sponsor and Reference
Systems Appl., Inc.	1978	Los Angeles	EPA, Contract RP-1375-1-2 (Seigneur et al., 1983)
Systems Appl., Inc./ State of Colorado	1973	Denver	Colorado Department of Highways, Contract 75-109
Systems Appl., Inc.	1976	Denver	EPA Region VIII, Contract 68-01-4341 (Anderson et al., 1977)
Systems Appl., Inc./ State of Colorado	1976	Denver	Colorado State Health Department and Department of Highways
Systems Appl., Inc.	1977	Denver	DOT, Contract DOT-FH-11-8529 (Reynolds et al., 1979)
Systems Appl., Inc.	1977	Denver	ERT/Colorado Interstate Pipline Company
Systems Appl., Inc.	1973	Las Vegas	EPA, Contract 68-03-2174 (Liu et al., 1977)
Systems Appl., Inc./ British Leyland	1973	Turin, Italy	British Leyland
Systems Appl., Inc.	1977	Phoenix	EPA, Contract 68-03-2446
Systems Appl., Inc.	1977	Tampa	EPA, Contract 68-03-2446
Systems Appl., Inc.	1978	St. Louis	EPA, Contract 68-02-2429
Systems Appl., Inc.	1978	St. Louis	EPRI, Contract RF-1375-1-2 (Seigneur et al., 1983)
Systems Appl., Inc.	1978	Sacramento	DOT, Contract DOT-FH-11-8529 (Reynolds et al., 1979)
Systems Appl., Inc.	1982	Las Vegas	Southern California Edison Company (Tesche, Oliver, and Haney, 1982)
SRI, International	1982	Philadelphia	EPA, Contract 68-02-3538
Systems Appl., Inc.	1983	Philadelphia	EPA, Contract 68-02-3582 (Haney, Tesche, and Killus, 1983)

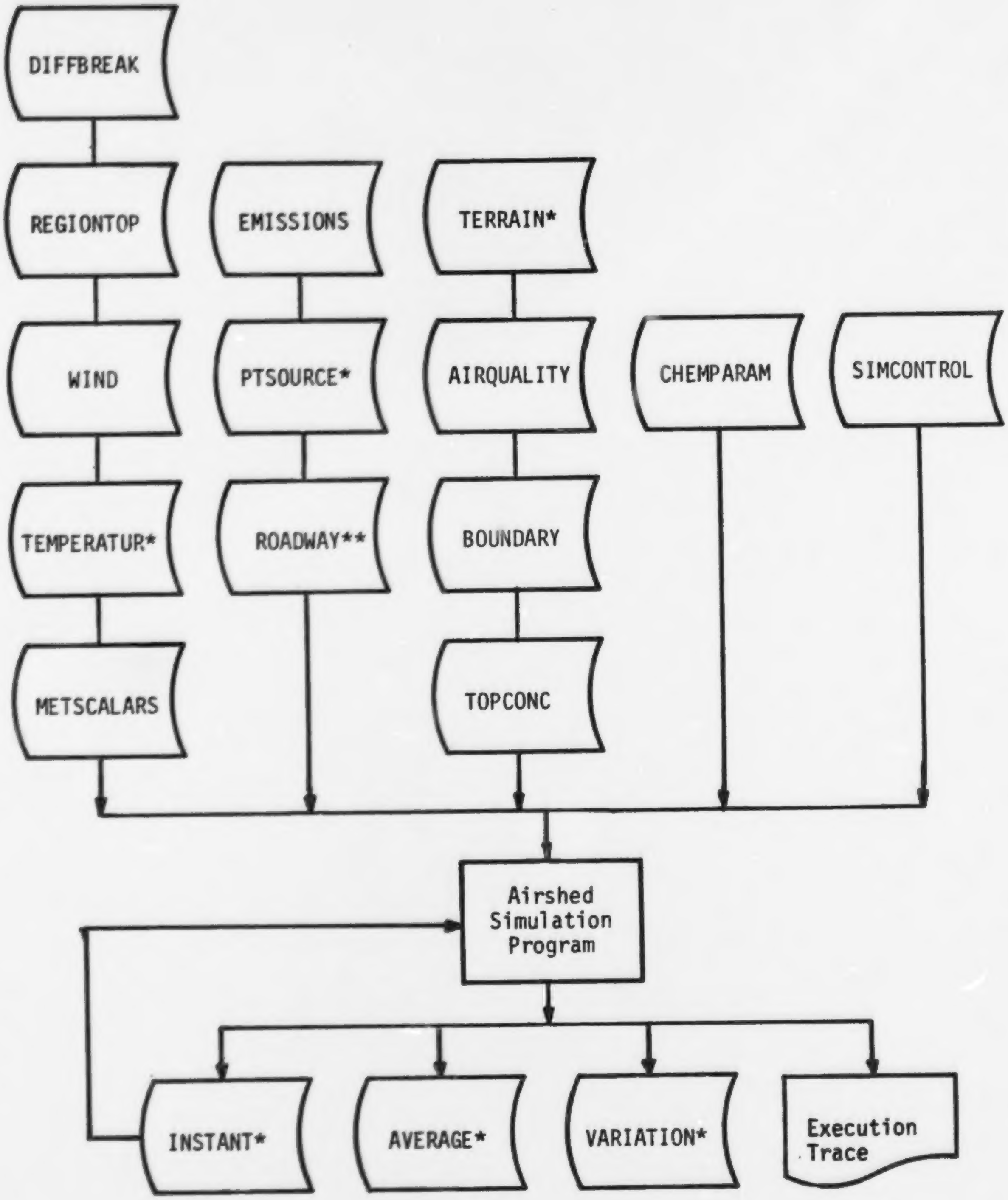
III OVERVIEW OF THE SYSTEM

The SAI Airshed Model System contains at its core the Airshed Simulation Program, the input data that consist of 10 to 14 files, depending on the program options chosen. Each file is created by a separate data preparation program. The output from the Airshed Simulation Program consists of three data results files and an execution trace report. The output data files can be further processed by the display and analysis programs and can also be used for restarting the simulation. Figure III-1 shows the Airshed Simulation Program and identifies its input and output files.

The SAI Airshed Model System can be described according to the five major tasks or functions that the user and the programs must perform:

> M.E.B. (meteorology, emissions, and initial and boundary conditions) file preparation.
> M.E.B. file segmentation.
> Control data preparation.
> Airshed simulation.
> Display and analysis.

This classification of programs and tasks is used as the organizational basis for both this User's Manual and the companion Systems Manual. Each of the five major functions is represented by a rectangular box in Figure III-2, which illustrates the flow of information through the system and shows the position of each major function within the system. The following sections of this chapter briefly discuss each function in terms of the activities required of the user, and the remaining chapters of this report present the detailed information necessary for the completion of each task.


DIFFBREAK
REGIONTOP
EMISSIONS
TERRAIN*
WIND
PTSOURCE*
AIRQUALITY
CHEMPARAM
SIMCONTROL
TEMPERATUR*
ROADWAY**
BOUNDARY
METSCALARS
TOPCONC
Airshed Simulation Program
INSTANT*
AVERAGE*
VARIATION*
Execution Trace

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* Optional files.

** Optional file not recommended for usage at this time.

Figure III-1. Airshed Simulation Program with Input and Output Files

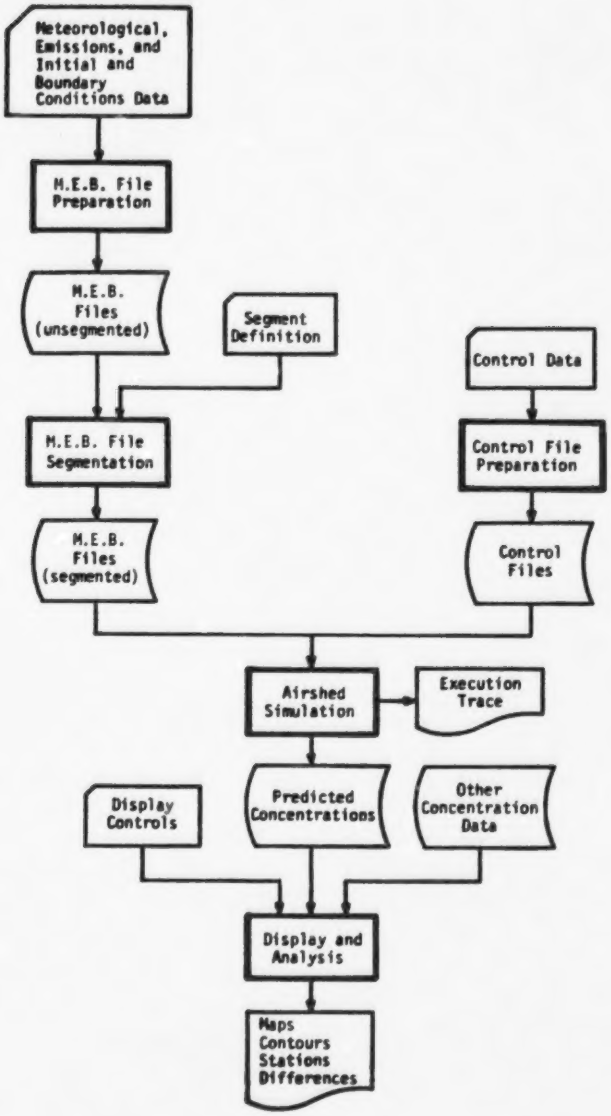

Meteorological, Emissions, and Initial and Boundary Conditions Data
M.E.B. File Preparation
M.E.B. Files (unsegmented)
Segment Definition
Control Data
M.E.B. File Segmentation
Control File Preparation
M.E.B. Files (segmented)
Control Files
Airshed Simulation
Execution Trace
Display Controls
Predicted Concentrations
Other Concentration Data
Display and Analysis
Maps
Contours
Stations
Differences

Figure III-2. Information Flow in the SAI Airshed Model System

A. M.E.B. DATA FILE PREPARATION

Of the 14 files input to the Airshed Simulation Program, two are classified as "control files" and are discussed separately. The preparation of the remaining 12 files, which contain meteorological, emissions, and initial and boundary conditions data (referred to in this report as the "M.E.B. files"), is discussed here. The Airshed Simulation Program requires appropriate meteorological, emissions, and initial conditions data for each cell of the region's rectangular grid. In addition, the concentration of each pollutant must be specified at each point on the boundary where the wind is flowing into the region. These data enter the program through the M.E.B. files. Table III-1 lists the 12 files, grouped by type; the 10-character code name as well as the descriptive name is given for each file. Also, the data items contained in each are listed and classified according to the nature of the variability (spatial, temporal, or pollutant) exhibited by each item.

For each file, there is a data preparation program that takes either observations or estimates at specific locations in the region, creates a fully gridded data field, and writes the data to the file in the appropriate format. The 12 M.E.B. data preparation programs are designed to be used together as a unified, user-oriented package. The input formats to all the programs are standardized and reasonably self-documenting. The interpolation methods are intended to accommodate input data of any complexity, from variables for which little or no data are available to those for which there are many observations and well-known interactions. Also, the units of measure are standardized, and a flexible unit conversion scheme is built into the programs.

The M.E.B. data preparation function consists of the following tasks for the user:

Table III-1. M.E.B. Data Files

	Nature of Variability			
File Description	Axes	Vertical Direction	Species	Time
Meteorological Files				
WIND--Wind				
$\lvert u\rvert^{\dagger}_{max}$, $\lvert v\rvert^{\dagger}_{max}$				t
Average wind speed along each boundary				t
u-velocity component	x y	z		t
v-velocity component	x y	z		t
DIFFBREAK--Diffusion Break				
Diffusion break	x y			t
REGIONTOP--Top of the Region				
Top of the modeling region	x y			t
*TEMPERATUR--Temperature				
Ground-level temperature	x y			t
METSCALARS--Meteorological Scalars				
Temperature gradient below diffusion break				t
Temperature gradient above diffusion break				t
Exposure index				t
Diurnal photolysis rate constant				t
Concentration of H_2O				t
Atmospheric pressure				t
Emissions Files				
EMISSIONS--Ground-Level Emissions				
Ground-level emissions (lumped mobile and nonpoint stationary sources)	x y		sp	t
*PTSOURCE--Point Source Emissions				
Location of source	(x,y)			
Effective plume height	(x,y)			t
Vertical cell index	(x,y)			t
Emissions rate	(x,y)	(z)	sp	t

Table III-1 (Concluded)

File Description	Nature of Variability			
	Axes	Vertical Direction	Species	Time
*ROADWAY--Roadway Microscale Parameters **				
Emissions from motor vehicles	x y		sp	t
Roadway microscale parameter	x y			t
Boundary Files				
*TERRAIN--Terrain Surface Parameters				
Surface roughness	x y			
Vegetation factor	x y			
BOUNDARY--Boundary Definition and Concentrations				
Boundary definition	(x,y)			
Boundary concentrations	(x,y)	z	sp	t
AIRQUALITY--Air Quality				
Initial concentrations	x y	z	sp	(t)§
TOPCONC--Concentrations at the Top of the Region				
Boundary concentrations at the top of the modeling region	x y		sp	t

---

x = east-west axis of grid.

y = north-south axis of grid.

z = vertical axis of grid.

sp = chemical species.

t = time.

() = data that vary spatially but are not present over the entire grid.

* = files that need not be present for a simulation run.

† u and v refer to the x and y components of the wind velocity, respectively.

§ Concentrations must be present at least for the beginning time of the simulation.

** = The roadway microscale procedure is not recommended for usage at this time.

> Determination of the appropriate files for a given simulation.

> Detailed examination of the data requirements and optional methods for each file.*

> Translation of available data into a form acceptable to the model.

> Selection of the proper interpolation methods.*

> Establishment of the size and location of the region.

> Establishment of the vertical distribution of cells within the region.

> Exercise of the data preparation programs, examination of the results, and modifications of the inputs or algorithms until a reasonable set of data is produced.

The preparation of the M.E.B. data files is certainly the most difficult and time-consuming task associated with using the SAI Airshed Model System. It is also the most important task, and careful, intelligent creation of the input is required to yield the best simulation results.

B. M.E.B. DATA FILE SEGMENTATION

The SAI Airshed Model System has been designed to enable simulation on a rectangular grid of any size and shape; that is, the dimensions of the region are not fixed within the programs, but are specified at run time. If a specified region does not fit within the core limitations of the host computer, that region can be divided into any number of contiguous subrectangles called "segments"; in this case, the size of each segment, rather than the size of the entire region, is limited by the amount of core available. The Airshed Simulation Program processes each segment in turn and information at the interfaces between segments is maintained.

---

* In some situations, the algorithms embedded in the data preparation programs may not be adequate for the intended model application; in these cases, the user will have to develop and interface the appropriate capability with the SAI Airshed Model System.

To enable simulation processing by segment, the user must create segmented data files from unsegmented files. The M.E.B. file segmentation function consists of the following tasks for the user.

- > Estimation of the size of the largest segment that will fit in core. This size will be determined by the number of species to be simulated, the number of vertical levels, the number of point sources, the program options selected, and the amount of core available on the host computer.
- > Definition of the size and arrangement of segments in the simulation region, and preparation of a segmentation control deck describing that layout.
- > Running the segmentation program on each of the spatially varying M.E.B. files.

C. CONTROL DATA PREPARATION

The Airshed Simulation Program requires two control files: the Chemistry Parameters file (CHEMPARAM), and the Simulation Controls file (SIMCONTROL), each created by its own data preparation program. Table III-2 summarizes the contents of the control files.

For the Chemistry Parameters file, all chemical species to be simulated are named and their properties specified. This list of species, rather than that appearing on any of the other data files, determines which species will be simulated. If there are any reactive species, the reaction rate constants and their other properties (such as the activation energy and reference temperature) are also specified. The user's tasks in making the Chemistry Parameters file are:

- > Preparation of a card deck describing the species and the chemical mechanism to be used.
- > Running the program that creates the Chemistry Parameters file.

TABLE III-2. Airshed Simulation Program Control Files

CHEMPARAM (Chemistry Parameters)

- For each species
  - Name
  - Reactivity flag
  - Steady-state flags
  - Lower and upper concentration bounds
- For each reaction
  - Rate constant
  - Photolysis and temperature-dependence flags
  - Activation energy and reference temperature
- For each coefficient
  - Name
  - Value

SIMCONTROL (Simulation Controls)

- Run identifier
- Beginning and ending times
- File options
- Simulation options
- Time slice controls
- Minimum chemistry time step
- Convergence criteria
- Averaging interval
- Instantaneous concentration output interval
- Print options

Note: These files contain no spatially or temporally variable parameters.

The Simulation Controls file includes values for the simulation options, time span, integration controls, and output options, which are the data likely to be changed most frequently. The user's tasks in generating this file are:

> Preparation of the card deck containing all the simulation control parameters.
> Running the program that creates the Simulation Controls file.

Although the creation of the Simulation Controls file is described as a separate task among a number of tasks preliminary to running the simulation program, it can be performed just prior to a simulation program run within the same computer job.

D. AIRSHED SIMULATION

The Airshed Simulation Program reads the data files that were created in the three previously described steps and performs the simulation as specified by the control files. Its output consists of files containing instantaneous and time-averaged concentration predictions in segmented form, and a printed trace of the progress of the simulation. Concentration predictions are not printed by the simulation program except in a compact form for debugging purposes only. The selective printing of the simulation results is performed by the display and analysis function. The user's tasks in running the airshed simulation are:

> Proper specification of all input files to be used.
> Arranging to save the output files that the program creates.

E. DISPLAY AND ANALYSIS

The final function of the SAI Airshed Model System is the display and analysis of the simulation results. This function has been removed from the Airshed Simulation Program because often, no matter which output options are selected for a simulation run, different options are needed at a later time. By writing the concentration predictions of all species in all dimensions to output files, one can select any available output mode at any later time.

The current display program capabilities include printout of either instantaneous or average concentration grid maps for selected species at selected vertical levels at selected times. Instantaneous or average vertical concentration profiles can also be printed at user-specified stations. The user's tasks in running the display program are:

> Proper specification of all input files required (including the desired output file from the Airshed Simulation Program).

> Preparation of an input deck containing parameters for the selection of times, species, and vertical levels to be printed, and station locations where vertical concentration profiles will be printed.

In addition, the design of the display program provides for the inclusion of additional analysis capabilities without extensive modification of the program. Specifically, the structure permits the comparison of two concentration data files. The two data files could be the output from two simulation runs (comparing different control strategies, for example), or one file could be simulation predictions and the other a gridded representation of station observation data.

IV DEFINITION OF SYSTEM CONCEPTS

This chapter discusses several important aspects of the Airshed Model System that must be understood before the model can be used. The concepts explained here include the subdivision of the modeling region into an array of three-dimensional grid cells, the pollutants treated by the model, and the handling of the time variability of various parameters in the model. Also, the segmentation of the entire modeling region into one or more subregions for performing the numerical integration process is examined. Finally, the treatment of time increments used in the Airshed Simulation Program is detailed.

A. THE MODELING REGION (GRID)

The modeling region is a three-dimensional volume subdivided into an array of three-dimensional grid cells. This section first describes the projection of this array onto the x-y, or horizontal, plane and then the method of determining the cell thicknesses in the z, or vertical, direction. Complete instructions for defining the location, size, shape, and resolution of the modeling region are given in Section VI.B.2, which discusses the REGION packet.

1. Horizontal Distribution of Grid Cells

Three pairs of values (which are further discussed below) define the horizontal modeling region:

> The x- and y-coordinates, in meters, of its origin (the lower left-hand corner point) with respect to a reference origin.

> The grid spacing (cell size), in meters, along each axis.
> The number of grid cells along each axis.

In the horizontal plane, the region consists of a rectangular grid area with the x-axis parallel to the equator (east-west) and the y-axis perpendicular to the equator (north-south).* This area is divided into rectangular grid cells of equal size. Although the spacing of cells may be different for one axis than for the other, yielding nonsquare cells, it must be uniform along each axis.

The region specified must include one cell at each boundary of the simulated area. Thus, if the area to be simulated is a 5 x 10 grid, the region specified must be at least 7 x 12, as shown in Figure IV-1. Also, portions of the inner rectangular area can be omitted from the simulation by defining the boundaries appropriately. Figure IV-2 shows a possible boundary for the Los Angeles region for which the prediction of concentrations in the areas over the Pacific Ocean and the San Gabriel Mountains would not be of interest. Boundaries of the simulated area are input to the simulation through the BOUNDARY file (see Section VI.A.6, which describes the method for defining the horizontal boundaries of the region).

The method for describing locations within the specified region has been standardized in the current version of the SAI Airshed Model. First, a "reference origin"--a point on the map defined by its Universal Transverse Mercator (UTM) coordinates--is designated. All other points in the region, including measuring stations, point sources, and the origin of the modeling region itself, are then described in terms of their distances in the x- and y-directions from the reference origin. The reference origin may coincide with the origin of the region, it may lie within the grid, or it may be completely outside the grid. Thus, the x- and y-coordinates of

---

* This orientation of the horizontal grid is used for reference throughout the system. However, some other more useful or convenient grid orientation can be used, provided that point locations and wind vector components are carefully defined.

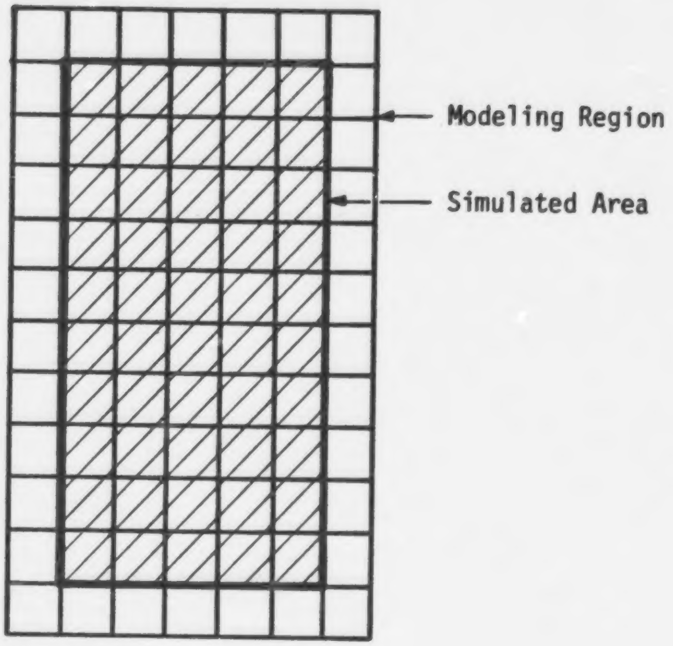

Modeling Region
Simulated Area

Figure IV-1. Example of a Modeling Region That Includes the Required Boundary Cells

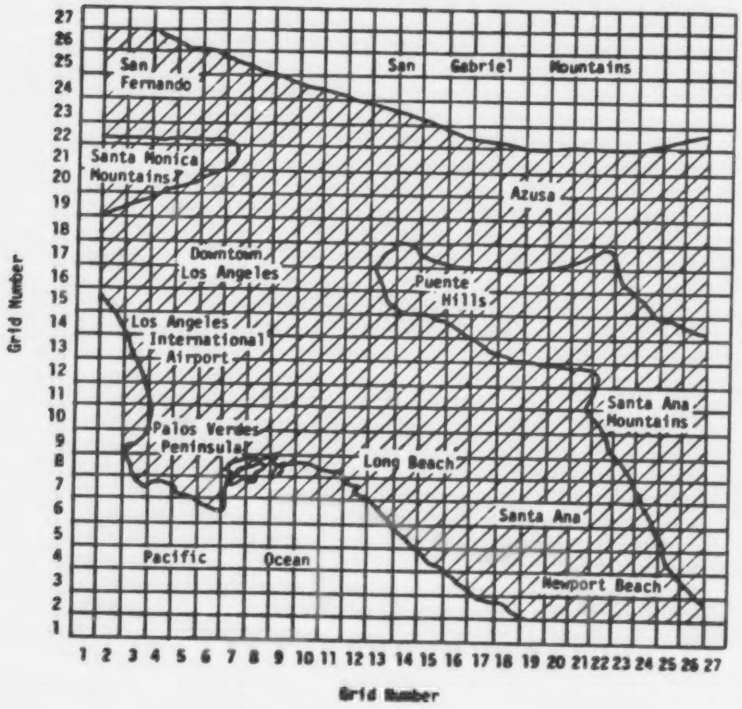

San Fernando
San Gabriel Mountains
Santa Monica Mountains
Azusa
Downtown Los Angeles
Puente Hills
Los Angeles International Airport
Santa Ana Mountains
Palos Verdes Peninsula
Long Beach
Santa Ana
Pacific Ocean
Newport Beach
Grid Number
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27
Grid Number
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27

Figure IV-2. 54 Mile by 54 Mile Modeling Region of Los Angeles Basin. Each grid square is 2 miles by 2 miles.

any point with respect to the reference origin may be positive or negative. In Figure IV-3, the reference origin is outside the modeling region. The x-coordinate of the region origin is positive and the y-coordinate is negative. The point sources and measuring stations appear both within the region and outside it. Using this method for locating points, the user can change the location, size, shape, or resolution of the modeling region without changing the coordinates of any of the other input data.

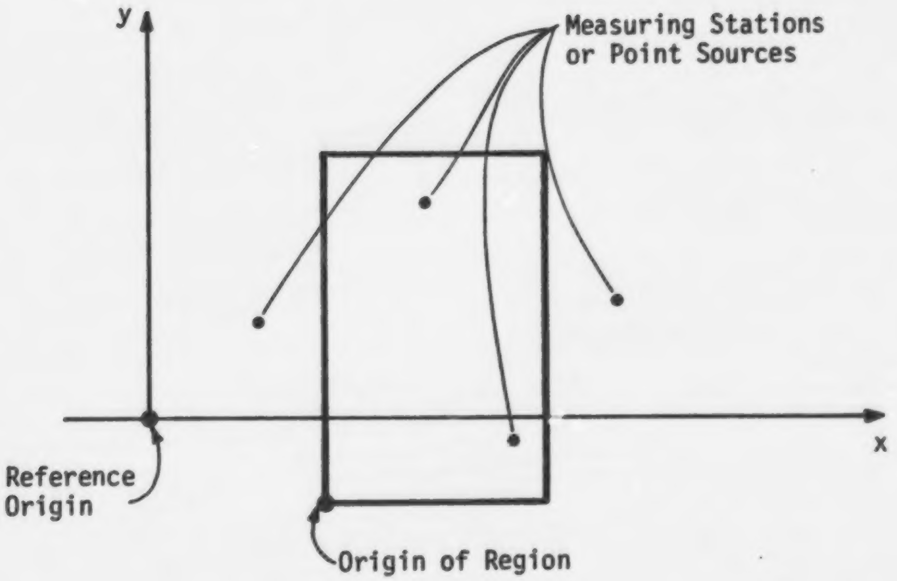

y
Measuring Stations
or Point Sources
x
Reference
Origin
Origin of Region

Figure IV-3. Example of the Location of a Modeling Region with Respect to a Reference Origin

It is sometimes necessary to describe the region in terms of its grid cells, generally when dealing with a whole cell (containing spatially averaged values) rather than a single point. Grid cell references instead of point locations are used to designate subregions and regional segments for the data preparation programs and to label printouts of grid values. Grid cells are numbered by their indices in the x- and y-directions, with Cell (1,1) referring to the cell in the lower left (southwest) corner of the grid, as illustrated in Figure IV-4.

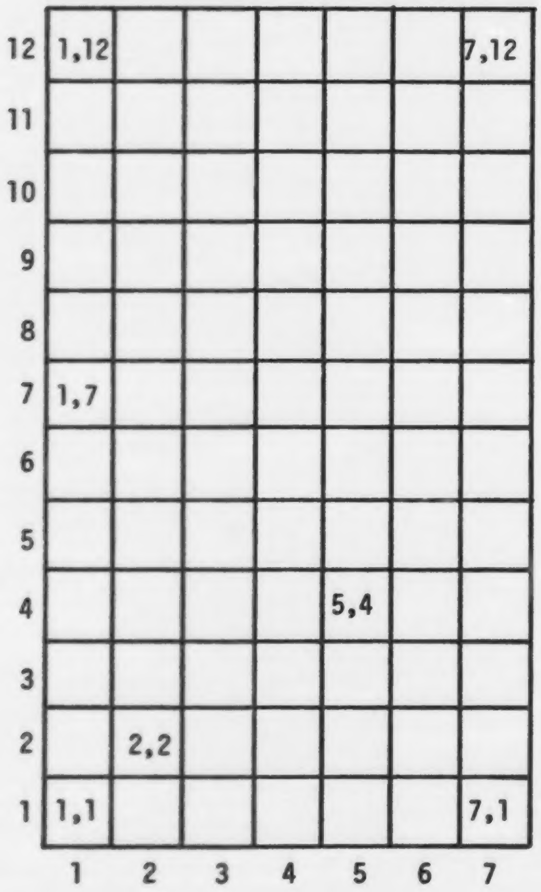


Figure IV-4. Conventional Method for Numbering Grid Cells

2. Vertical Distribution of Grid Cells

Although the modeling region in the horizontal plane consists of rectangular cells of equal size, cells in the vertical direction are distributed differently. The vertical distribution of cells is described using the following definitions:

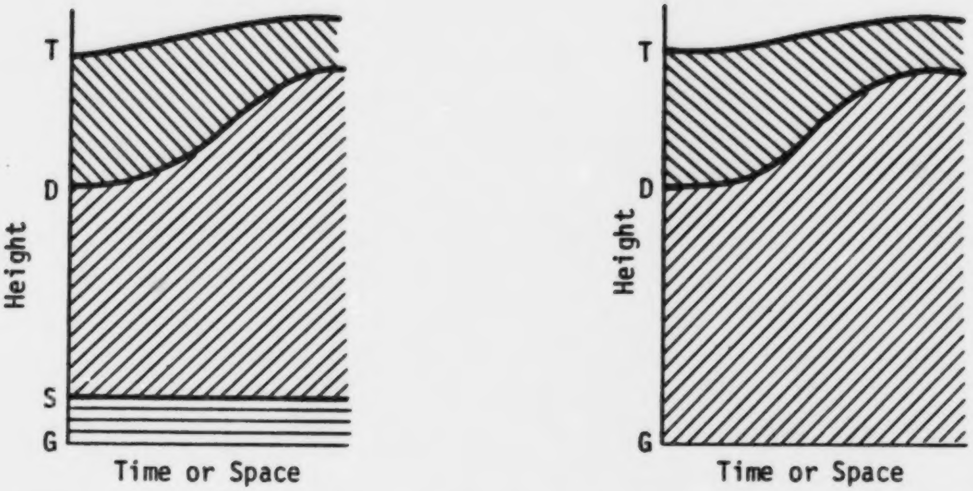
- The diffusion break is the height above ground at which the diffusion characteristics (or eddy diffusivity) undergo a significant change. For example, when a mixed layer is capped by a stable inversion layer, the diffusion break occurs at the base of the inversion. If a ground-based stable layer is present, the diffusion break then occurs at the top of the inversion layer. Gridded values of the diffusion break are specified as a function of x, y, and time, and are input via the file DIFFBREAK.
- The top of the region is the height above ground of the top of the simulation region. Gridded values are specified as a function of x, y, and time, and are contained in the file REGIONTOP. The top of the region may be located below, above, or at the same height as the diffusion break.
- The space between the ground and the top of the region is divided into three layers:
  - The surface layer is one cell deep, and all surface layer cells maintain a constant height over space and time. Microscale calculations are performed in this layer using concentration predictions from the corresponding cell immediately above each surface layer cell. Ground-level emissions, surface deposition, and the reaction products of NO emissions from roadways and ambient ozone are combined to produce a flux of each pollutant into the cell above the surface layer cell. If the surface layer height is set to

zero, there is no surface layer and the microscale calculations are bypassed. Since the microscale prediction capabilities have not been fully tested, it is recommended that the surface layer height be set to zero.

- The lower layer, which must be at least one cell deep, includes the cells between the top of the surface layer (or those at ground level, if there is no surface layer) and the diffusion break.
- The upper layer includes the cells between the diffusion break and the top of the region. Calculations in this layer can be omitted by setting its number of cells to zero.

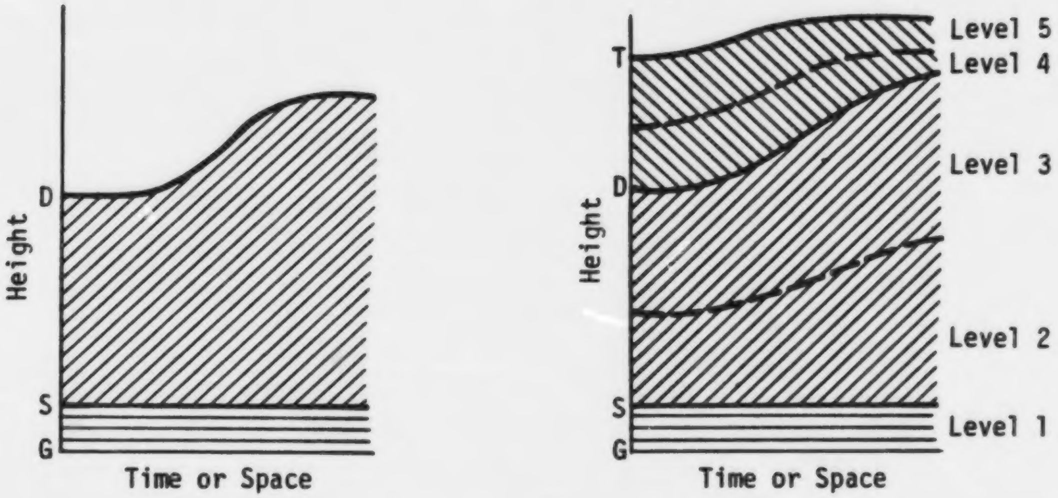
Figure IV-5 illustrates various "layer" configurations that can be employed in the model. Figure IV-5(a) shows surface, lower, and upper layers. Figure IV-5(b) omits the surface layer. Figure IV-5(c) contains surface and lower layers, but no upper layer; note that, in this case, the top of the region actually modeled is the diffusion break, not the region top parameter input. The user must specify the number of cells and the minimum cell height in the lower and upper layers. Figure IV-5(d) shows the region described in Figure IV-5(a) with two cells in the lower layer and two cells in the upper layer. The number of levels in the region, i.e., the number of cells in the vertical dimension of the concentration matrix, is equal to the number of cells in the lower layer plus the number of cells in the upper layer plus one, if there is a surface layer. The total number of levels is used to calculate the segment size limitation. For example, five levels are described in Figure IV-5(d).

If either the lower or upper layer cells (as defined above) are smaller than the minimum cell height specified, enough space is borrowed from the adjacent layer to make up that height. Such a situation occurs in cases in which the diffusion break is very low or it is higher than the top of the region. Figure IV-5(e) illustrates all possible vertical cell distributions for a region that embodies a surface layer, two cells in the lower layer, and two cells in the upper layer. The top of the region is assumed to be high enough to include the total number of cells


T
D
Height
S
G
Time or Space
T
D
Height
G
Time or Space

(a) Configuration of a Region into Surface, Lower, and Upper Layers

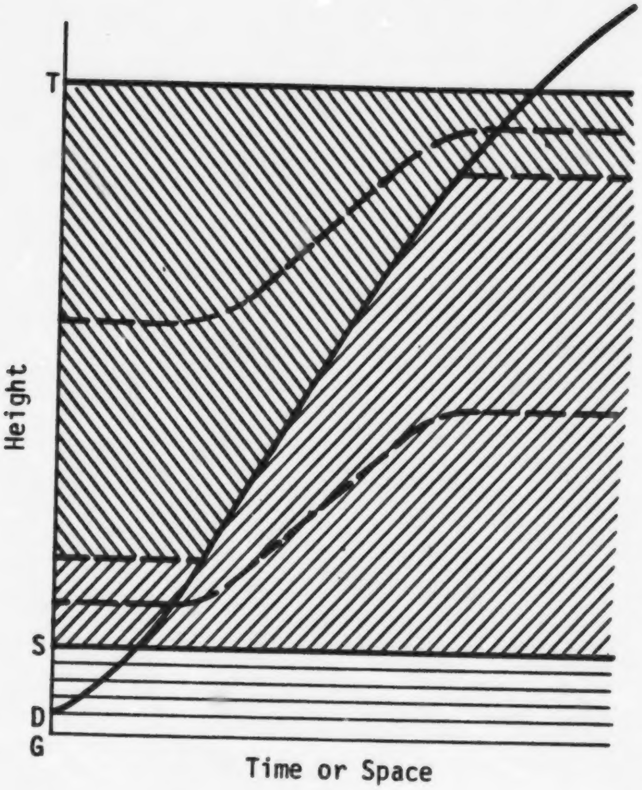
(b) Configuration of a Region into Lower and Upper Layers


D
Height
S
G
Time or Space
T
D
Height
S
G
Time or Space
Level 5
Level 4
Level 3
Level 2
Level 1

(c) Configuration of a Region into Surface and Lower Layers

(d) The Region Described in Figure IV-5(a) Sectioned into Five Levels

Figure IV-5. Various Vertical Cell Distributions That Can Be Employed in the SAI Airshed Model



(e) All Possibilities for Vertical Cell Distribution of a Region That Contains a Surface Layer and Two Cells Each in the Upper and Lower Layers

G = Ground.

D = Diffusion break.

S = Height of the surface layer.

T = Top of the region.

☰ Surface layer.

▨ Lower layer.

▧ Upper layer.

Figure IV-5 (Concluded)

at the minimum height. For cases in which the minimum cell height is used to create a pseudo-lower layer or a pseudo-upper layer, the simulation program still uses the actual height of a cell with respect to the diffusion break rather than the cell number to calculate the vertical diffusivity. Instructions for specifying the vertical distribution of cells in the region are given in Section VI.B.2, which discusses the REGION packet.

B. CHEMICAL SPECIES

Each cell in the three-dimensional region previously described will carry a concentration value for each chemical species simulated. The Chemistry Parameters (CHEMPARAM) file indicates the species to be considered and their properties (Section IX.A). Initial concentrations of each pollutant are provided by the Air Quality (AIRQUALITY) file. The vertical column of concentrations at each boundary cell of the horizontal plane are provided by the Boundary (BOUNDARY) file. Boundary concentrations for each species at the top of the region are on the Top Concentrations (TOPCONC) file. Instructions for creating these three files are given in Chapter VII.

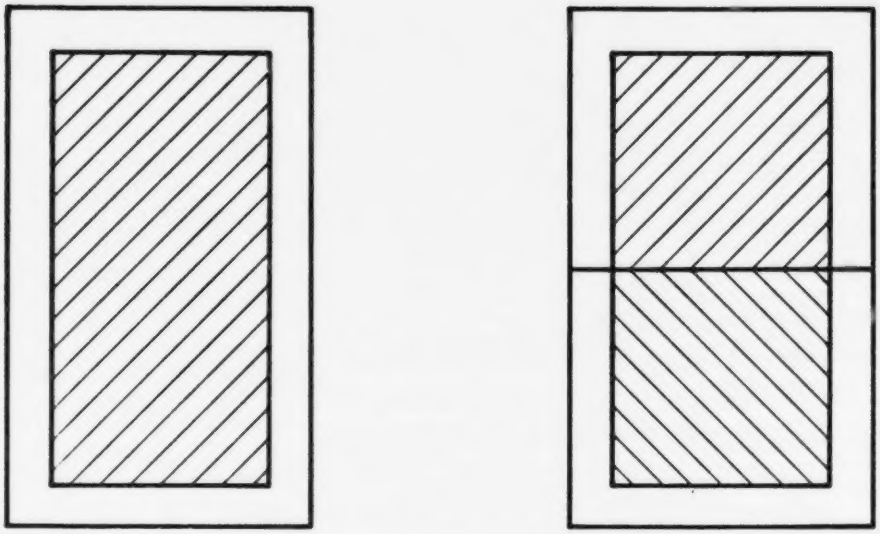
C. TIME

Concentrations of each species in each cell are moved ahead from a beginning time to an ending time in increments called "time slices". The beginning time, ending time, and the size of time slice are specified on the Simulation Controls (SIMCONTROL) file (Section IX.B). The time intervals for concentration averaging and for the output of the four-dimensional concentration fields are also specified on this file. A further discussion of the treatment of time is given in Section E of this chapter.

D. SEGMENTATION

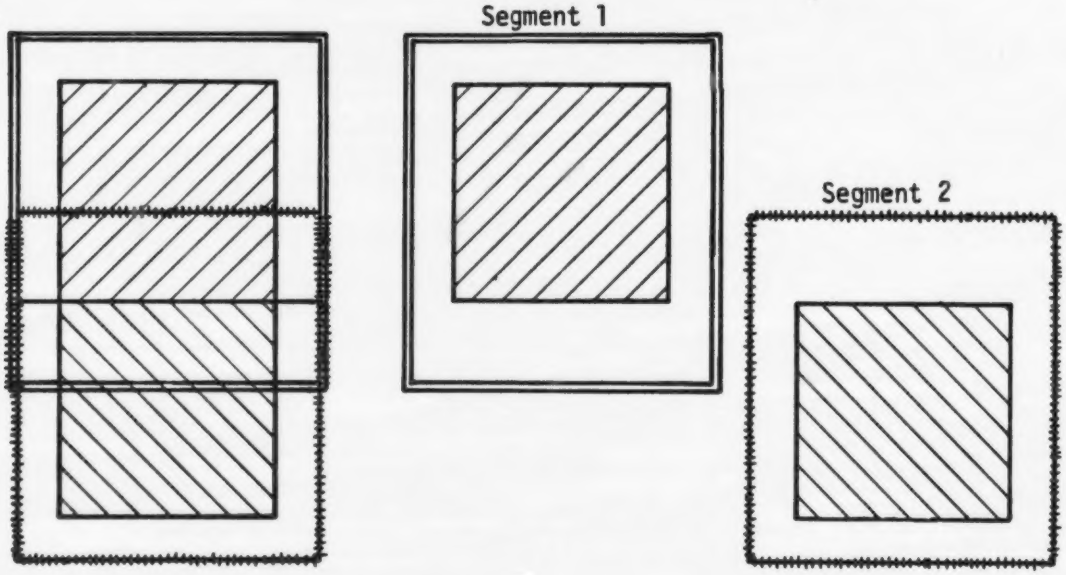
The segmentation process involves dividing the user-defined modeling region into one or more rectangular segments in the horizontal plane, thereby allowing the Airshed Simulation Program to retain in core the data for the entire area it is processing, and providing flexibility as to the choice of the number and size of grid cells. The maximum horizontal dimensions for each segment are determined by the amount of core storage available on a particular computer, the number of vertical levels and chemical species to be simulated, and the simulation options to be used. Although the data arrays for all segments are maintained in secondary storage, all of the data arrays for a single segment reside in core during the period that the segment is being processed.

Each segment must be constructed as if it were an independent region being simulated, with its own set of input data and boundary conditions. To provide adequate information at the segment interfaces, adjacent segments must be constructed with a four cell overlap, as illustrated in Figures IV-6(a) through IV-6(c). Figure IV-6(a) shows a 7 x 12 cell region, consisting of a 5 x 10 area to be simulated plus a one-cell boundary on all edges. If the data covering this area do not fit in core, the area can be divided into two segments as shown in Figure IV-6(b). However, since each segment must include two boundary cells from the adjacent segment, the length of each segment is increased by two cells at the interface boundary. Figure IV-6(c) shows the layout of the original region, segmented into two 7 x 8 regions, each with a 5 x 5 simulation area. The two southernmost simulated rows of Segment 1 are the north boundary cells for Segment 2, and the two northernmost simulated rows of Segment 2 are the south boundary cells of Segment 1. Instructions for calculating maximum segment size and defining the regional segment layout are given in Chapter VIII.



(a) A 5 x 10 Cell Region with a One-Cell Boundary on All Edges

(b) Division of the 5 x 10 Cell Region into Two 5 x 5 Cell Segments



(c) Layout of a Region Showing the Interface of Boundary Cells for Two Segments

Figure IV-6. Example of the Segmentation of a Region

E. TIME SLICES AND INTEGRATION TIME STEPS

The "time slice" is the amount of simulation time during which the integration for any segment will proceed without updating the boundary conditions or any other time-varying data. At the beginning of a time slice, new data from the files are read if necessary, and the concentrations at the segment interfaces are updated (Chapter VII of the Systems Manual details the method of maintaining segment interface concentrations). Then, each segment in turn is entirely processed for one time slice. Because all data for a given segment are in core at once, this scheme reduces the number of I/O transfers.

To describe how the time slice is determined, another time increment--the integration time step--must be defined. The integration time step is the increment over which the numerical integration of the governing equations in a segment actually takes place. The numerical integration procedure consists of four sequential steps:

- Horizontal advection and diffusion (Steps 1 and 2).
- Vertical advection and diffusion, including the treatment of emissions, surface deposition, and the surface layer microscale effects (Step 3).
- Chemistry (Step 4).

The maximum time step allowable for the horizontal transport calculations in a segment is determined by the simulation program on the basis of the maximum wind velocity component over the segment and by the horizontal grid cell size:

$$\Delta t_{max} = \min\left(\frac{.5\Delta x}{|u|_{max}} \quad , \quad \frac{.5\Delta y}{|v|_{max}}\right) \quad ,$$

where

Δt_{max} = maximum allowable time step for the segment,
Δx = size of the grid cell in the x-direction,
Δy = size of the grid cell in the y-direction,
$|u|_{max}$ = maximum absolute value of the wind velocity component in the x-direction over the entire segment for all vertical levels,
$|v|_{max}$ = maximum absolute value of the wind velocity component in the y-direction over the entire segment for all vertical levels.

The size of the time slice is determined in the following way:

> First, the time slice is set to the maximum size input by the user on the SIMCONTROL file.

> If necessary, the time slice is reduced to avoid exceeding the time interval for which the data on any input file apply.

> Also, if necessary, it is further reduced to avoid exceeding the next output time (instantaneous or average).

> Finally, it is reduced if necessary on the basis of the smallest maximum time step that is allowed in any segment.*

---

* The user sets the maximum number of time steps that can be taken in any slice. Thus, the time slice used can be no larger than

$$n(\Delta t_{max})_{min} \quad ,$$

where n = maximum number of steps in a slice (input on the SIMCONTROL file), and $(\Delta t_{max})_{min}$ = the smallest maximum allowable time step calculated for any segment. In general, if n is set large, the time slice used will be limited by the maximum time slice input. If n is small, the time slice used will be limited by the smallest allowable time step for any segment.

After the size of the time slice has been determined, the overall integration time step to be used for each segment is calculated. If the maximum time step for the segment is shorter than the calculated time slice, the slice is divided into the smallest number of equal time steps such that each is less than or equal to the maximum time step. Thus, if the time slice is 0.25 hour, and the maximum time step is 0.10 hour, the time slice is divided into three equal time steps of 0.08 1/3 hours each. If the maximum time step is greater than the time slice, the overall time step used will be equal to the time slice.

The overall time step described above (limited by the maximum wind speed and time slice size) may still be too large to allow completion of the chemistry step (Step 4). If the time step used for advection is too large to allow convergence in the chemistry calculations for any given cell, the time step is cut in half only for the chemistry step for that cell. This "chemistry time step" is successively halved until the chemistry calculations converge, and a sufficient number of these steps are taken for that cell to fill out the overall time step. If the chemistry time step for any cell must be decreased to less than the minimum chemistry time step specified by the user (on SIMCONTROL), the simulation will stop and values of all arrays will be printed in the neighborhood of the cell.

V JOB CONTROL SPECIFICATIONS

This manual does not present specific job control examples because they vary greatly depending not only on the computer system used but also on the intentions and the style of the individual user. Instead, Chapters VII through XI contain diagrams illustrating the flow of information (card decks, binary files, and printed output) among the various computer programs. This chapter discusses a typical information flow diagram, suggests a worksheet for keeping track of programs, and provides a summary of file characteristics to aid in the preparation of job control statements.

A. INFORMATION FLOW DIAGRAMS

Each information flow diagram provides the following details, which are specified for each program being described:

- The names of the files associated with the program
- The FORTRAN unit number assigned to each file
- The program name
- Any necessary subroutine libraries
- Any optional flow patterns.

Figure V-1 is an example of such a diagram. The input is a card deck read on Unit 5 (the standard read unit), and a binary file named BINARY, read on Unit 3. An optional input file--BIN2--if present, is read on Unit 2. The program to be executed--PROGM--requires subroutines that are stored in SUBLIB. The output from the program is another binary file called BINOUT, written on Unit 4, and a printout of results on Unit 6, the standard print unit.

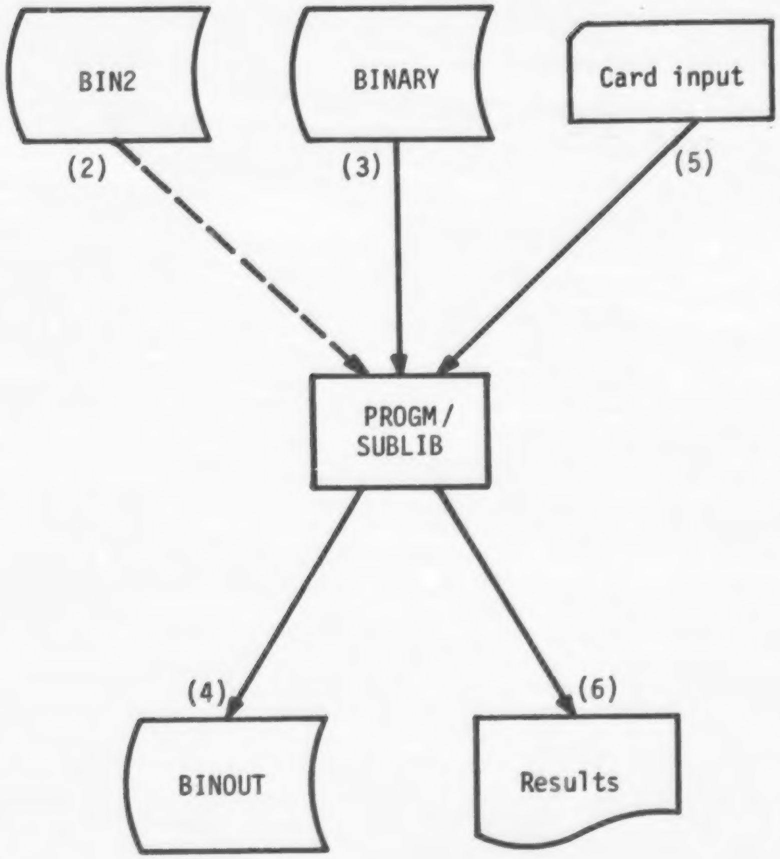

BIN2
BINARY
Card input
(2)
(3)
(5)
PROGM/
SUBLIB
(4)
(6)
BINOUT
Results

Figure V-1. Example of an Information Flow Diagram for Use in Job Control

B. PROGRAM WORKSHEET

This manual assumes that the programs have already been compiled and that they exist in an executable form. Exhibit V-1(a) is a worksheet that can be used to locate and identify each program in the system; Exhibit V-1(b) shows that worksheet filled out for use on the Lawrence Berkeley Laboratory (LBL) system. To use a different system, users who implement the programs must provide the information necessary to run them, including link/loading information, storage requirements, and the location of predefined procedures.

C. FILE CHARACTERISTICS

The 17 data files associated with the SAI Airshed Model are described in detail in Chapter IX of the Systems Manual. This section simply tabulates the essential features of each file to aid in the preparation of job control statements.

With the exception of the card-image input files and the output print files, all files in the SAI Airshed Model are binary (unformatted) files of variable record lengths. Each file contains one to four standard header records followed by data records specific to the particular file. The following terms are used to express the number of records on a file and the maximum record length:

sg = number of segments,
sp = number of species,
x_{max} = largest number of cells in the x or y dimension for any segment,
xy_{max} = largest number of grid cells in the horizontal plane for any segment,
z = number of vertical levels,
pt_{max} = largest number of point sources in any segment.

Program	Source	Object	Libraries	Scratch Vector	Size	Other Information
AIRQUL						
BNDARY						
DIFFBK						
EMISSN						
METSCL						
PTSRCE						
REGNTP						
ROADWY						
TMPRTR						
TERAIN						
TOPCON						
WNDSET						
UTILITY						
FILUTIL						
SEGDEF						
CPREP						
SPREP						
AIRSIM						
DISPLAY						

(a) Format

Exhibit V-1. Sample SAI Airshed Model Program Worksheet for Use in Job Control

Program	Source	Object	Libraries	Scratch Vector	Size	Other Information
AIRQUL	AIRQULU	AIRQUAL	U, F	14,500	170000_8	
BNDARY	BNDARYU	BOUNDRY		17,000		
DIFFBK	DIFFBKU	DIFFBRK		26,500		
EMISSN	EMISSNU	EMISSON		20,000		
METSCL	METSCLU	METSCAL		40,000		
PTSRCE	PTSRCEU	PSOURCE		23,500		
REGNTP	REGNTPU	REGNTOP		22,500		
ROADWY	ROADWYU	ROADWAY		20,000		
TMPRTR	TMPRTRU	TMPRTUR		26,500		
TERAIN	TERAINU	TERRAIN		27,000		
TOPCON	TOPCNCU	TOPCONC		20,000		
WNDSET	WINDSTU	WINDSET		11,900		
UTILITY	UTILTYU	UTILITY		—	—	
FILUTIL	FILUTLU	FILUTIL		—	—	
SEGDEF	SGMTDFU	SGMTDEF			—	
CPREP	JCPREP	JCPREPR	—	—	$32,000_8$	
SPREP	JSPREP	JSPREPR	—	—	$27,000_8$	
AIRSIM	JSIMU	JSIMR	—	30000	$170,000_8$	Overlay form -- requires AUTOLAY control deck
DISPLAY	DISPLAY		—	—	134000_8	

(b) Worksheet Filled Out for Use on the LBL System

Exhibit V-1 (Concluded)

Table V-1 shows the number of words in each of the four header records. Table V-2 lists the 17 files, indicates the number of records appearing on each one, and gives the maximum length of a nonheader record. If this length is smaller for the largest segment than that of the longest header record, then the longest header determines the maximum record length for the whole file. In addition to the 17 data files shown in Table V-2, some temporary scratch files might be used by a particular program, depending on the implementation and the size of the region to be modeled. Chapter IX of the Systems Manual explicitly defines these files.

Table V-1. Header Record Lengths for the SAI Airshed Model Data Files

Record Name	Length (decimal words)
File description header record	76
Region description header record	15
Segment description header record	4 sg
Species description header record	10 sp

Table V-2. Characteristics of the SAI Airshed Model Data Files

Name of File	Header Records				Number of Time-Invariant Records	Number of Records per time Interval	Maximum Data Record Length (decimal words)
	File	Region	Segment	Species			
AIRQUALITY	✓	✓	✓	✓	--	1 + sg*sp*z	$11 + xy_{max}$
BOUNDARY	✓	✓	✓	✓	4sg	1 + 4*sg*sp	$12 + x_{max}*z$
DIFFBREAK	✓	✓	✓		--	1 + sg	$11 + xy_{max}$
EMISSIONS	✓	✓	✓	✓	--	1 + sg*sp	$11 + xy_{max}$
METSCALARS	✓	✓			--	2	66
PTSOURCE	✓	✓	✓	✓	2sg	1 + sg*(2 + sp)	6*pt 11 + pt
REGIONTOP	✓	✓	✓		--	1 + sg	$11 + xy_{max}$
ROADWAY						1 + sg*(1 + sp)	$11 + xy_{max}$
TEMPERATUR	✓	✓	✓		--	1 + sg	$11 + xy_{max}$
TERRAIN	✓	✓	✓		2sg	--	$11 + xy_{max}$
TOPCONC	✓	✓	✓	✓	--	1 + sg*sp	$11 + xy_{max}$
WIND	✓	✓	✓		--	1 + 2sg*z	$11 + xy_{max}$
CHEMPARAM	✓			✓	2-4	--	62 18 sp 5*reactions 11*coefficients
SIMCONTROL	✓				1	--	36
AVERAGE	✓	✓	✓	✓	--	1 + sg*sp*z	$11 + xy_{max}$
INSTANT	✓	✓	✓	✓	--	1 + sg*sp*z	$11 + xy_{max}$
VARIATION	✓	✓	✓	✓	--	1 + sg*sp	$11 + xy_{max}$

VI PACKETS USED IN CREATING THE M.E.B. FILES

As many as 12 different data preparation programs are required for constructing the M.E.B. files--one program for each file. This chapter discusses the data modules--packets--that are used by the data preparation programs. All input data are divided into packets; each packet contains a specific type of information necessary to some aspect of data preparation. The following sections first present general rules that apply to the preparation of all the packets, and then explicit rules and formats for each one. Chapter VII contains rules for the preparation of the data files using these packets, and examples of the output from the programs.

A. ELEMENTS OF PACKET CONSTRUCTION

The ordering and internal structure of the data packets have been designed for consistency of formats, flexibility of use, and ease of visual analysis. Each packet begins with a header card identifying the packet and ends with a termination/trailer card that reads END or ENDTIME. The packet names, their classifications, and their proper ordering are shown in Table VI-1.

Of the time-invariant data, the CONTROL and REGION packets are mandatory, and they are entered first and second, respectively, in the input deck. The CONTROL packet defines input and output options and maximum variable counters used by the program to set internal array dimensions. The REGION packet defines the location, size, and resolution of the modeling region. If present, the UNITS packet follows the REGION packet. The UNITS packet names user-defined variables and specifies unit conversions.

Table VI-1. Packets Used by the SAI Airshed Model Data Preparation Programs

Time-Invariant Packets

- CONTROL
- REGION
- UNITS
- STATIONS
- POINT SOURCES
- BOUNDARIES

Time-Varying Packets

- TIME INTERVAL
- SUBREGIONS
- METHOD
- VERTICAL METHOD
- CONSTANTS
- GRID VALUES
- STATION READINGS
- EMISSIONS VALUES
- EMISSIONS FACTORS
- BOUNDARY READINGS
- SCALARS
- VERTICAL PROFILES

The remaining time-invariant packets, STATIONS, BOUNDARIES, and POINT SOURCES, which define fixed locations in the region, are optional depending on the file being created and the method used.

The TIME INTERVAL packets appear next. Each TIME INTERVAL packet contains the other time-varying packets to be used during the interval specified and ends with an ENDTIME card. The time intervals used must cover the time span specified in CONTROL with no gaps or overlaps. The time-varying packets included within each TIME INTERVAL packet define the data preparation methods to be used and supply the time-varying data.

Different interpolation methods can be used for different variables in different areas of the region. The SUBREGION packet defines the areas, and the METHOD packet defines the method to be used for each variable in each subregion. The VERTICAL METHOD packet describes the method to be used for calculating values for variables that vary vertically. Although any of these packets can be changed in subsequent time intervals, for most runs the subregions and methods supplied in the first time interval will be used for the entire duration of the run. The other time-varying packets define the values for the input variables. The particular packets used for any given run depend on the file being created and the methods selected. After the first TIME INTERVAL packet has defined the information to be written on the file, this information will persist into succeeding time intervals as described in Section A.3 of this chapter.

1. Rules for Card Format

Each data card is divided into two sections: Columns 1 to 60 contain input data; Columns 61 to 80 are reserved for any desired user identification information. All input fields are 10 columns wide except packet headers and file identifiers, which can occupy the entire width available for input, i.e., Columns 1 to 60.

Integers are input in Format I10 and must be right justified. Floating point variables are input as F10.0. Alphanumeric information can occupy any of the columns available for input of that data as long as it is correctly ordered and no extraneous or erroneous symbols are included. Thus, for example, _C_ON__TROL___ would be recognized as "CONTROL"; CNOTROL and CONTROLZ would not. The 60-column file identifier is not subject to validation and, therefore, can contain any information the user desires.

2. The Reserved Word ALL

The word ALL is a special designation that is reserved to enable the user to specify information globally; therefore, it should not be used to indicate a specific alphanumeric entity, such as a variable, subregion, station, point source, or boundary name. When used in the input field usually associated with an alphanumeric name, ALL means that the subsequent information applies to all the names that could occupy that input field. ALL can generally be used wherever it makes sense. The following examples illustrate both the proper and improper usages of this command:

> Proper usages of ALL.

- A card in the METHOD packet:

|ALL _______|__WX______|GRIDVALUE| .

This card specifies that in all subregions the values of the variable WX will be input by the GRID VALUE method. If ALL also occurred in place of WX, e.g.,

|ALL_______|ALL_______|GRIDVALUE| ,

the values of all input variables in all subregions would also be input by the GRID VALUE method.

- A card in the STATION READINGS packet:

  |WEST______|__ALL_____|-9.0______| .

  This information indicates that the values of all variables reported by Station WEST are to be set to -9.0 (a value that implies data are missing).

> Improper usage of ALL. A card in the UNITS packet:

|ALL_______|KG/D______|a |b |c | ,

where a, b, and c are numbers. This card says that all input variables will have values input in kg/day, to which the conversion parameters a and b and the molecular weight c are to be applied. It is improper because different species have different molecular weights.

3. Persistence of Data

As previously mentioned, the information provided in any TIME INTERVAL packet remains in effect until it is replaced. This persistence rule applies to all time-varying data, including subregion and method definitions and input values. For example, METHODs for computing each variable in each subregion need be specified only in the first TIME INTERVAL. They can be changed in a later TIME INTERVAL if desired, but in most cases only one definition is required.

If no data are available for a given station over a certain time interval, the user can omit that station in that time interval, and the data previously input will be used. However, if the data are actually to be treated as missing, the station must be included and must be assigned values that are interpreted by the program as "missing data." In general, missing integer and real values are represented by -9 and -9.0, respectively. Although the use of this device can save considerable duplication of effort, it places on the user the burden of ensuring that all changes in status are specified.

4. Units of Measure

The Airshed Simulation Program assumes a standard and consistent set of units for all of its computations, and the files input to the program must contain data expressed in these "internal" units. The data input to the file preparation programs, however, may be in other than internal units. To accommodate such data, the programs contain a set of standard alternative unit designations for use in directing automatic conversion of input units to internal units. Additionally, the user can specify the use of nonstandard conversion factors. Section B.3 of this chapter discusses the internal units for each variable, alternative units and their associated conversion factors, and the method for specifying nonstandard unit conversions.

5. Variables

Each program has a set of output variables. For files that vary by species, the output variables are the species names listed in the CONTROL packet. For files that do not vary by species, the output variables are names built into the corresponding data preparation program; the implicit output variable names for each file are presented in the appropriate section of Chapter VII. Values input to the program may be for the output variables themselves, or they may be for variables that will be acted on in some way to produce the output variables. For example, concentrations of total hydrocarbon may be input to the AIRQUALITY program, whereas its output consists of concentrations in each of several carbon-bond classes.

Whenever the input variables are different from the output species or implicit output variables, they are referred to as "user-defined variables," and must be named in the UNITS packet. Designation of the user-defined variables in this way allows the program to allocate space for them internally.

6. Methods

This section explains the methods for calculating the ground-level values of each variable within each subregion. (Section B.8 of this chapter gives instructions on dividing the modeling region into subregions.) These methods are designated in the METHOD packet, which is discussed in Section B.9 of this chapter. The first eight methods (a through h) can be used by any of several data preparation programs; the remaining methods (i through r) are each specific to a single program.

a. CONSTANT

A single value is to be used for this variable in every ground-level cell in this subregion. The value must be defined in a CONSTANTS packet and the program will convert it to internal units if necessary. The CONSTANT method requires no other parameters.

b. GRID VALUE

A value for this variable will be input for each ground-level grid cell in the subregion. The values will be defined in a GRID VALUES packet and the program will convert them to internal units if necessary. The GRID VALUE method requires no other parameters.

c. STATINTERP (Station Interpolation)

The value for this variable at each ground-level grid cell in the subregion is calculated by the program as the weighted average of values at selected measuring stations. Station locations will be defined in a STATIONS packet; values for the variable at each station will be input in the STATION READINGS packet and the program will convert them to internal units if necessary. To calculate the value at a given grid cell, the program weights each station value by the inverse of the distance of the station from the center of the cell. The following four parameters must be specified to control the selection of the measuring stations to be included in the average:

> EXTENT--This number determines the acceptability of a station on the basis of the subregion it is in. If EXTENT = 0.0, a station within the radius of influence will be included in the average regardless of the subregion it occupies. If EXTENT ≠ 0.0, only stations within the same subregion will be accepted. If this number is omitted, it will be assumed to be zero.

> INITRADIUS--initial radius of influence. All stations within this distance of the cell for which values are being calculated will be used. This number is assumed to be in grid units. If this number is set very large, all stations will be included. Omission of this number constitutes an error.

> RADIUSINCR--If no measuring stations with values are encountered within the initial radius of influence, the radius will be incremented by this amount until at least one station is included. This number is assumed to be

in grid units. When this number is small, the values generated will be distributed more smoothly over the region, but the cost in computing time could be great. Conversely, when this number is large, computing time might be reduced, but at the expense of irregularities in the computed grid values. If this number is omitted, only the initial radius will be used, and the failure to find a valid station constitutes an error.

> MAXRADIUS--maximum radius of influence. This number is assumed to be in grid units. Failure to find valid station data within this radius constitutes an error. If this number is omitted, the entire modeling region may be used.

d. POISSON

The value for this variable at each ground level grid cell in the subregion is calculated by the program using the Poisson smoothing method [see Killus et al. (1977), Chapter IV, pp. 135-142]. Values for the variable at selected measuring stations must be input in the STATION READINGS packet. The POISSON method requires three parameters:

> MAXITER--the maximum number of iterations; the suggested number is $\leq$ 200.

> ERRORTOL--error tolerance. This parameter is expressed in internal units of the variable; the suggested value = 0.01 * expected value.

> OMEGA--weighting factor to aid convergence; the suggested value = 1.4.

e. SPLIT/COMB (Split or Combine)

Any variable to be output can be formed by splitting or combining input variables (typically, these are species):

$$var_{out} = \sum_{i=1}^{N} var_{i} * factor_{i} \quad .$$

This method requires N parameter cards; on Card i the parameter name is the name of $variable_i$ and the value is $factor_i$. If the parameter (variable) name is left blank, the corresponding factor is treated as a constant (i.e., $var_i = 1$). All values for input variables will already have been converted to internal units when this computation is done, so the factors specified should not include unit conversions.

f. E-W INTERP (East-West Interpolation)

For each row of grid cells within a subregion, a linear interpolation will be carried out between values in the bordering cells in the east and west edges of the row. This subregion must not lie on an edge (i.e., it must be bounded on east and west by other subregions) and values for the bordering subregions must be calculated by a noninterpolative method. The E-W INTERP method requires no other parameters.

g. N-S INTERP (North-South Interpolation)

For each column of grid cells within a subregion, a linear interpolation will be carried out between values in the bordering cells on the north and south edges of the column. This subregion must not lie on an edge (i.e., it must be bounded on north and south by other subregions), and values for the bordering subregions must be calculated by a noninterpolative method. The N-S INTERP method requires no other parameters.

h. USER (User-Supplied Algorithm)

Each data preparation program is designed to call a user-supplied subroutine for any variable for which the method USER has been selected. All available data are passed to the subroutine as arguments. At present, all user subroutines are dummies; as new methods are developed, they can be inserted in user subroutines, and parameter values can be read and passed as for any of the standard methods.

i. BOUNDVALUE

This method is used only for creation of the BOUNDARY file. It specifies that concentration values will be input for each boundary line segment through the BOUNDARY READINGS packet. BOUNDVALUE requires no parameters.

The following two methods are used only for creating the PTSOURCE file.

j. EMVALUES

This method name indicates that point source emissions will be entered for this species for this point source type (the "subregion" field) by means of the EMISSIONS VALUES packet. EMVALUES requires no parameters.

k. EMFACTORS

This method name indicates that for this species and point source type, the emissions values and flow rate previously entered will be modified by factors supplied by means of an EMISSIONS FACTORS packet. This method requires no parameters.

The following two methods are used only for the REGIONTOP file. Both require that the DIFFBREAK file be input and that the vertical definition of the region be included in the REGION packet. Both use NZUPPR (the number of cells in the upper layer) as defined in the REGION packet.

1. FIXDHEIGHT

The REGIONTOP is defined such that there will be NZUPPR cells of a fixed height above the diffusion break, subject to the maximum height indicated on the method card. REGIONTOP can be defined as being equal to the diffusion break, subject to the maximum height indicated on the method card, by specifying NZUPPR = 0. This method requires one parameter: UPCELLHT--the cell height in the upper layer (above the diffusion break). If NZUPPR > 0, this number must be specified and must be greater than the minimum height of upper layer cells.

m. SAMEHEIGHT

The REGIONTOP is defined such that there will be NZUPPR cells above the diffusion break of the same height as the NZLOWR cells between the top of the surface layer and the diffusion break, subject to the maximum height indicated on the method card. No other parameters are required.

The following two methods are used only for the TOPCONC file. Both require that vertical concentration profiles be input by means of a VERTICAL PROFILES packet; i.e., they require that for each species in each subregion, a number of height-concentration pairs be provided. Both methods require the REGIONTOP file. The method RELTOPCONC requires the DIFFBREAK file as well.

n. ABSTOPCONC

The concentration at the top of the region will be calculated from the profile based on the height of the top of the region. The vertical profile input describes the vertical distribution of concentration values. The height of the top of the region above ground is compared with the height of each profile point to determine the value to be used. The profile is input as a set of pairs (H_i, F_i), where H is height and F is some profile value. Since it is assumed that the pair (H_1, F_1) corresponds to ground level, the following transformation is applied to all heights:

$$H_i' = H_i - H_1 \quad .$$

The profile is thus considered to be the set of pairs (H_i', F_i) ordered by increasing H'.

The profile is used for a particular grid cell in the following way: For a cell at a given (x,y) location on the grid, find the height T of the top of the region. Then, the concentration, C, at the top is defined as follows:

$$C = \begin{cases} F_n \text{, if } T > H_n' & ; \\ F_{i-1} + \dfrac{T - H_{i-1}'}{H_i' - H_{i-1}'}\left(F_i - F_{i-1}\right) \text{, if } H_{i-1}' \le T \le H_i' & . \end{cases}$$

o. RELTOPCONC

The concentration at the top of the region will be calculated from the profile based on the height of the top of the region relative to the height of the diffusion break. The vertical profile input describes the vertical distribution of concentration values. The height of the top of the region relative to the height of the diffusion break is compared to the height of each profile point relative to its diffusion break to determine the value to be used. The profile is input as a set of pairs (H_i, F_i), where H is height and F is some profile value. Since it is assumed that the pair (H_1, F_1) corresponds to ground level, the following transformation is applied to all pairs: For all i,

$$H_i' = (H_i - H_1)/DB_p \quad ,$$

where DB_p = diffusion break at the profile location. The profile is thus considered to be the set of pairs (H_i', F_i) ordered by increasing H'.

The profile is used for a particular grid cell in the following way. For a cell at a given (x,y) location on the grid, find the height of the top of the region. Then, convert the absolute height T to the height of the top relative to the diffusion break at that location:

$$T' = \frac{T}{DB} \quad .$$

Then, the concentration, C, at the top is defined as follows:

$$C = \begin{cases} F_n \text{ , if } T' > H_i' & ; \\ \\ F_{i-1} + \dfrac{T' - H_{i-1}'}{H_i' - H_{i-1}'} \left(F_i - F_{i-1}\right) \text{ , if } H_{i-1}' \le T' \le H_i' & . \end{cases}$$

The following three methods are used only in the WIND program. In this program there are four implicit variables: SPEED and DIRECTION, the variables ordinarily input to the program; and WINDX and WINDY, the x- and y-components of the wind that are written to the WIND file. Further discussion of the specification of these variables appears in Chapter VII.

p. DIVERGENCE

The DIVERGENCE method uses the algorithms developed by Anderson and Durran and reported in Killus et al. (1977) to calculate a three-dimensional wind field. The method is unique in that it calculates the values for the two output variables (WINDX and WINDY) simultaneously and computes the values for all cells at all levels. DIVERGENCE is, therefore, also a vertical method and must be explicitly named in the VERTICAL METHOD packet as well. Use of this method requires that station readings and vertical profiles for SPEED and DIRECTION be specified and that the ground-level temperature field (TEMPERATUR data file) be available. Since this method internally performs a Poisson interpolation, it requires the same three parameters as the POISSON method (previously discussed). These parameters should be specified for the first variable (WINDX or WINDY) that appears using the DIVERGENCE method. The other variable (WINDY or WINDX) should also use the DIVERGENCE method, but no parameter need be included. The vertical method for both of these variables should also be DIVERGENCE. This method cannot be specified for SPEED or DIRECTION. The DIVERGENCE method requires that the files DIFFBREAK, REGIONTOP, and TEMPERATUR be attached to the run.

The methods VECTORIZE and POLARIZE are used only to calculate the three-dimensional arrays. Necessary conversion of station values and profile values are handled automatically.

q. POLARIZE

This method can only be specified for the variables SPEED and DIRECTION. The values of SPEED and DIRECTION will be calculated from the vector components WINDX and WINDY. This method should be used if printouts of gridded SPEED and DIRECTION are desired. Some method other than VECTORIZE (discussed next) should be specified for WINDX and WINDY if POLARIZE is used. No parameters are required.

r. VECTORIZE

This method is used to convert SPEED and DIRECTION to WINDX and WINDY. This method should be used to calculate the output variables WINDX and WINDY if gridded SPEED and DIRECTION values are given or calculated by the program. POLARIZE should not be the method used for SPEED and DIRECTION if VECTORIZE is used for WINDX and WINDY.

7. Vertical Methods

The vertical methods are used to define values of the output variables at each vertical cell, given the values at ground level. Each method assumes that ground-level values already exist and are in internal units. These methods are designated in the VERTICAL METHOD packet, which is discussed in Section B.10 of this chapter. The first eight vertical methods (a through h) can be used by any of several data preparation programs; the remaining methods (i through k) are each specific to a single program.

a. CONSTANT

Values in each vertical cell are equal to the ground-level value. This method requires no additional parameters.

There are four vertical methods that require the input of a vertical profile to describe the shape of the vertical distribution of values. These vertical methods require that the DIFFBREAK and REGIONTOP files be attached. For two of these methods, ABSPROFILE and RELPROFILE, the ground-level value only is used in calculating vertical distribution. For the other two, ABSPROFRAT and RELPROFRAT, the value for the variable at the top of the region is required in addition to the ground-level value, and the profile defines the shape of the interpolation between them. These two ratio methods also require the TOPCONC file.

Each of these general vertical profile methods can be used in either the "absolute" or "relative" mode. In the absolute mode, the heights provided with each profile point are directly used to calculate the variable value at a cell of a given height. That is, the absolute height of the cell above ground is used to determine the profile value. In the relative mode, the heights provided with each profile point are used as heights relative to the diffusion break or top of region at the specified location of the profile.

b. ABSPROFILE

The vertical profile input describes the shape of the vertical distribution of values using the ground-level value. The height of each cell above ground is compared with the height of each profile point to determine the scaling factor to be used. The profile is input as a set of pairs (H_i, F_i), where H is height and F is some profile value. Since it is assumed that the pair (H_1, F_1) corresponds to ground level, the following transformation is applied to all pairs:

$$H_i' = H_i - H_1 \quad ,$$

$$F_i' = F_i/F_1 \quad .$$

The profile is thus considered to be the set of pairs (H_i', F_i') ordered by increasing H'.

The profile is used for a particular grid cell in the following way: For a cell at a given (x,y) location on the grid, find the average height (A_k) of each vertical cell (k) as a function of the diffusion break and top of the region. If the ground-level value at that location is V_1, then

$$V_k = \text{factor}_k{*}V_1 \quad ,$$

where

$$\text{factor}_k = \begin{cases} F_n' \text{, if } A_k > H_n' & ; \\ F_{i-1}' + \dfrac{A_k - H_{i-1}'}{H_i' - H_{i-1}'}\left(F_i' - F_{i-1}'\right) \text{, if } H_{i-1}' \le A_k \le H_i' & . \end{cases}$$

c. RELPROFILE

The vertical profile input describes the shape of the vertical distribution of values using the ground-level value. The height of each cell relative to the height of the diffusion break is compared to the height of each profile point relative to its diffusion break to determine the scaling factor to be used. The profile is input as a set of pairs (H_i, F_i), where H is height and F is some profile value. Since it is assumed that the pair (H_1, F_1) corresponds to ground level, the following transformation is applied to all pairs: For all i,

$$H_i' = (H_i - H_1)/DB_p \quad ,$$

$$F_i' = F_i/F_1 \quad ,$$

where DB_p = diffusion break at profile location. The profile is thus considered to be the set of pairs (H_i', F_i') ordered by increasing H'.

The profile is used for a particular grid cell in the following way. For a cell at a given (x,y) location on the grid, find the average height A_k of each vertical cell k as a function of the diffusion break and top of the region. Then convert the absolute height A_k to the height of the cell relative to the diffusion break at that location:

$$A_k' = \frac{A_k}{DB} \quad .$$

If the ground-level value at that location is V_1, then

$$V_k = \text{factor}_k * V_1 \quad ,$$

where

$$\text{factor}_k = \begin{cases} F_n' , & \text{if } A_k' > H_n' \quad ; \\ \\ F_{i-1}' + \dfrac{A_k' - H_{i-1}'}{H_i' - H_{i-1}'}\left(F_i' - F_{i-1}'\right), & \text{if } H_{i-1}' \le A_k' \le H_i' \quad . \end{cases}$$

d. ABSPROFRAT

The vertical profile input describes the shape of the vertical distribution of values expressed as the relative contribution (weighting) of the ground-level value and another value (which may be the value at the top of the region). The height of each cell above ground is compared with the height of each profile point to determine the contribution factor to be used. The profile is input as a set of pairs (H_i, F_i), where H is height and F is a profile value $0 \leq F \leq 1$. $F = 0$ means that the ground-level value only should be used. $F = 1$ means that the other (top) value only should be used. (The exact formula is shown below.) Since it is assumed that the pair (H_1, F_1) corresponds to ground level, the following transformation is applied to all heights: For all i,

$$H'_i = H_i - H_1 \quad .$$

The profile is thus considered to be the set of pairs (H'_i, F_i) ordered by increasing H'.

The profile is used for a particular grid cell in the following way. For a cell at a given (x,y) location on the grid, find the average height A_k of each vertical cell k as a function of the diffusion break and top of the region. If the ground-level value at that location is V_g and the other (top) value is V_t, then

$$V_k = V_g + \text{factor}_k \, (V_t - V_g) \quad ,$$

where

$$\text{factor}_k = \begin{cases} 1.0 \text{ , if } A'_k > H'_n \quad ; \\ \\ F'_{i-1} + \dfrac{A'_k - H'_{i-1}}{H'_i - H'_{i-1}} \left(F'_i - F'_{i-1}\right) \text{ , if } H'_{i-1} \leq A'_k \leq H'_i \quad . \end{cases}$$

e. RELPROFRAT

The vertical profile input describes the shape of the vertical distribution of values expressed as the relative contribution (weighting) of the ground-level value and another value (which could be the value at the top of the region). The height of each cell relative to the diffusion break is compared to the height of each profile point relative to its diffusion break in order to determine the contribution factor to be used. The profile is input as a set of pairs (H_i, F_i), where H is height and F is a profile value, $0 \leq F \leq 1$. $F = 0$ means that the ground-level value only should be used. $F = 1$ means that the other (top) value only should be used. (The exact formula is presented below.) Since it is assumed that the pair (H_1, F_1) corresponds to ground level, the following transformation is applied to all heights: For all i,

$$H_i' = (H_i - H_1)/DBp \quad ,$$

where DBp = diffusion break at profile location. The profile is now considered to be the set of pairs (H_i', F_i) ordered by increasing H'.

The profile is used for a particular grid cell in the following way. For a cell at a given (x,y) location on the grid, find the average height A_k of each vertical cell k as a function of the diffusion break and top of the region. Then convert the absolute height A_k' to the height of the cell relative to the diffusion break at that location:

$$A'_k = \frac{A_k}{DB} \quad .$$

If the ground-level value at that location is V_g and the other (top) value is V_t, then

$$V_k = V_g + \text{factor}_k \, (V_t - V_g) \quad ,$$

where

$$\text{factor}_k = \begin{cases} 1.0 \text{ , if } A'_k > H'_n \quad ; \\ \\ F'_{i-1} + \dfrac{A'_k - H'_{i-1}}{H'_i - H'_{i-1}} \left(F'_i - F'_{i-1}\right) \text{ , if } H'_{i-1} \le A'_k \le H'_i \quad . \end{cases}$$

f. E-W INTERP (East-West Interpolation)

For each row a linear interpolation will be carried out between values in the bordering cells in the east and west edges of the row. This subregion must not lie on an edge (i.e., it must be bounded on east and west by other subregions), and values for the bordering subregions must be calculated by a noninterpolative method. The E-W INTERP method requires no other parameters.

g. N-S INTERP (North-South Interpolation)

For each column a linear interpolation will be carried out between values in the bordering cells on the north and south edges of the column. This subregion must not lie on an edge (i.e., it must be bounded on north and south by other subregions), and values for the bordering subregions must be calculated by a noninterpolative method. The N-S INTERP method requires no other parameters.

h. VERTUSER (User-Supplied Algorithm)

For each file containing vertically varying data, the file preparation program is designed to call a user-supplied subroutine for any variable for which the vertical method VERTUSER has been selected. All available data are passed to the subroutine as arguments. At present, all vertical user subroutines are dummies; as new methods are developed, they can be inserted in user subroutines, and parameter values can be read and passed as for any of the standard vertical methods.

To create the PTSOURCE file, a vertical method must be chosen for determining the height at which the emissions from each point source enter the modeling region. Two vertical methods have been provided: STACKHGT and PLUMERISE, described below. Each of these vertical methods requires that the DIFFBREAK and REGIONTOP files be attached to the run.

i. STACKHGT

The emissions enter the region in the vertical cell that contains the top of the stack. No additional parameters are required.

j. PLUMERISE

Plume rise is calculated by the Briggs formulae [see Briggs (1975)]. For this vertical method the TEMPERATUR, METSCALARS, and WIND files must also be attached to the run. PLUMERISE requires no other parameters.

k. DIVERGENCE

The vertical method DIVERGENCE is used only for the WIND file. If DIVERGENCE has been specified in the METHOD packet for WINDX and WINDY, it must also be specified in the VERTICAL METHOD packet for those variables. No other parameters are required.

B. PACKET RULES AND FORMATS

This section presents the following information for each packet:

- Instructions as to where the packet is used.
- Special information about the contents.
- A table outlining the definition of each field on the cards.
- An exhibit showing the appearance (format) of the packet as a whole.

1. CONTROL Packet Rules

The CONTROL packet must always be the first packet input. The first three cards are the packet header, and the name and identifier of the file to be created. The next five cards contain counters for dimensioning arrays, and input and output option specifications; the standard entries are listed in Table VI-2. These control parameters are used in different combinations for different programs; each file preparation description in Chapter VII includes a table of the specific control parameters required for each file. For some files, some control parameters do not apply; these parameters are listed as "Spare" and any values are ignored. Following the control cards are those containing species names, if any, and the time span of the file. The contents of each card in the CONTROL packet are described in Table VI-3, and the format is shown in Exhibit VI-1.

Table VI-2. Standard Entries for Cards 4 Through 8 of the CONTROL Packet for M.E.B. Files

Card Number	Entries
4	Number of species
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Number of vertical parameters
	Number of heights in profile
	Print vertical methods table
	Print vertical profile tables
	Spare
	Spare
8	DIFFBREAK file number
	REGIONTOP file number
	TOPCONC file number
	TEMPERATUR file number
	METSCALARS file number
	WIND file number

Table VI-3. CONTROL Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be CONTROL, left adjusted
2 File Name	File name 1-10	10A1	--	Must be the name (type) of the file to be created; misspellings will not be tolerated
3 File Identifier	Identifier 1-10	60A1	--	Can be any alphanumeric sequence; it will not be validated, but will be written on the file and used in printed page headings exactly as given
4-8				These cards contain integer-format control information; all five cards must be included for all programs even though a given program does not require all the control information
4 Control Counters				
	Number of species 1-10	I10	--	For files that vary by species, this is the number of species output to the file; for files that do not vary by species, this number should be zero; in either case, this parameter controls the number of species names read from Cards 9+ in this packet; for files that do not vary by species, the species names are ignored

Table VI-3 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
	Number of user-defined variables 11-20	I10	--	If species are input that do not appear in the output list, their number must be provided here; they must also be named in the UNITS packet; for files that do not vary by species, there is no need for user-defined variables by any of the current methods; if a user-defined method requires other than the standard variables, however, the additional variables can be enumerated here and named in the UNITS packet, and values can be supplied in the time-varying data packets
	Number of stations (or boundary lines or point sources) 21-30	I10	--	Defines the maximum number of fixed locations in the region that are to be specified in time-invariant packets
	Number of subregions 31-40	I10	--	Maximum number of different subregions that will be named in all SUBREGION packets; must be at least one
	Number of parameters 41-50	I10	--	Maximum number of parameters that are defined or implied for all methods in all subregion-variable pairs; to obtain this value, multiply the number of parameters required for each method by the number of subregion-variable pairs that use the method (ALL counts not as 1, but as the total number); each time a parameter is redefined, it must be counted as a separate entry; add 3 to the maximum number of entries to ensure that enough space is allocated

Table VI-3 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
5 Output Controls				
	Output file unit number 1-10	I10	--	Depending on the implementation, a specific number may be required for each output file
	Input print option 11-20	I10	--	= 0--don't print cards; = 1--do print input cards
	Output print option 21-30	I10	--	= 0--don't print all output data; = 1--do print all output data
6 Print Options				For all options specified on this card, the value 0 means "don't print it" and the value 1 means "do print it"
	Print units table 1-10	I10	--	
	Print station locations (or boundaries or point sources) 11-20	I10	--	
	Print region 21-30	I10	--	
	Print methods table 31-40	I10	--	
	Print station values (or boundary values or point source emissions) 41-50	I10	--	

Table VI-3 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
7 Vertical Controls				Meaningful only for files that vary vertically; for other files, this card should be blank
	Number of vertical parameters 1-10	I10	--	Maximum number of parameters that are defined or implied for all vertical methods for all subregion-variable pairs; this value is computed in the same manner as the number of parameters (defined on Card 4)
	Number of profile heights 11-20	I10	--	Maximum number of height-value pairs that will be input for any single profile
	Print vertical methods table 21-30	I10	--	= 0--don't print it; = 1--do print it
	Print vertical profiles table 31-40	I10	--	= 0--don't print it; = 1--do print it
8 File Unit Assignment			--	Contains FORTRAN unit numbers for files that might be required as input to a particular data preparation program; if any of these files is not to be read in a run, its field should be left blank or set to zero; for consistency, the same unit number should be assigned to a given file for every data preparation program using that file

Table IV-3 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
	DIFFBREAK unit number 1-10	I10	--	Suggested value = 11, if required
	REGIONTOP unit number 11-20	I10	--	Suggested value = 12, if required
	TOPCONC unit number 21-30	I10	--	Suggested value = 13, if required
	TEMPERATUR unit number 31-40	I10	--	Suggested value = 14, if required
	METSCALARS unit number 41-50	I10	--	Suggested value = 15, if required
	WIND unit number 51-60	I10	--	Suggested value = 16, if required
9+ Species Names	Species 1-10	10A1	--	One species name per card; the number of species cards to be included here is defined on Card 4

Table VI-3 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
10 Time Span				Defines the time span for which the file contains data; this card must be present
	Beginning date 1-10	I10	Julian date (yyddd)	yy is the last two digits of the year and ddd is the three-digit Julian date
	Beginning time 11-20	I10	Military time (hhmm)	hh is hours and mm is minutes--this time will be internally converted to hours and fraction
	End date 21-30	I10	Julian date (yyddd)	Same format as that for beginning date
	End time 31-40	I10	Military time (hhmm)	Same format as that for beginning time
11 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	CONTROL						60A1
2	File Name	File name						10A1
3	File Identifier							60A1
4	Control Counters	# species	# u-def var	# stn	# subreg	# param	spare	6I10
5	Output Controls	output file	pr input	pr output	spare	spare	spare	6I10
6	Print Options	pr units	pr stn loc	pr region	pr meth	pr stn val	spare	6I10
7	Vertical Controls	#vert param	# heights	pr vert meth	pr vert prof	spare	spare	6I10
8	File Unit Assignments	DIFFBREAK unit #	REGIONTOP unit #	TOPCONC unit #	TEMPERATUR unit #	METSCALARS unit #	WIND unit #	6I10
9+	Species Names	spec name						10A1
10	Time Span	beg date	beg time	end date	end time			4I10
11	Packet Terminator	END						10A1

Exhibit VI-1. CONTROL Packet Format

2. REGION Packet Rules

The REGION packet must follow the CONTROL packet. It contains a complete definition of the location, size, and resolution of the modeling region. The same REGION packet values should be used to prepare all M.E.B. files for a given region. The contents of each card in the REGION packet are described in Table VI-4 and the format is shown in Exhibit VI-2.

Table VI-4. REGION Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be REGION, left adjusted
2 Reference Origin (UTM)				The origin (in UTM coordinates) used to locate the modeling region and all other fixed points (stations, point sources, boundary lines); these numbers are not used for computation but are compared to the reference origins on other files for consistency
	x-location 1-10	F10.0	m	x-coordinate
	y-location 11-20	F10.0	m	y-coordinate
	Zone 21-30	I10	--	UTM zone
3 Origin of Grid				The location of the lower left-hand corner of the grid with respect to the reference origin; this point is used to place the grid on the map; the grid is assumed to be rectangular and is oriented with the x-direction increasing to the east and the y-direction increasing to the north; the grid origin may be the same as the reference origin, in which case the coordinates are 0.0, 0.0
	x-location 1-10	F10.0	m	x-coordinate
	y-location 11-20	F10.0	m	y-coordinate

Table VI-4 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
4 Grid Cell Size				The grid consists of a matrix of rectangular cells of the same size and shape; this card defines the length of the cell along each axis
	x-size 1-10	F10.0	m	x-length
	y-size 11-20	F10.0	m	y-length
5 Grid Size				Defines the size of the grid in terms of the number of cells in each horizontal direction and the number of cells in the vertical direction
	Number of cells in x-direction 1-10	I10	--	Must be > 0
	Number of cells in y-direction 11-20	I10	--	Must be > 0
	Number of cells in z-direction 21-30	I10	--	Should be equal to the number of cells in the lower layer, plus the number of cells in the upper layer, plus one if there is a surface layer of nonzero height (see Card 6); for files that do not vary vertically, this number can be set to 0
6 Vertical Definition				Contains the parameters required to define the vertical distribution of cells within the region; (see Section IV.A.2 for a detailed discussion of vertical distribution parameters); if the number of z cells = 0, this card must be present, but the values will be ignored

Table VI-4 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
	Number of cells in lower layer 1-10	I10	--	Must be ≥ 1
	Number of cells in upper layer 11-20	I10	--	Must be ≥ 0
	Surface layer 21-30	F10.0	m	Height of surface layer; must be 0.0 if no surface layer is to be simulated (since microscale features have not been fully tested, set to 0.0)
	Lower layer 31-40	F10.0	m	Minimum height of cells in lower layer
	Upper layer 41-50	F10.0	m	Minimum height of cells in upper layer
7 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	REGION						60A1
2	Reference Origin (UTM)	x-loc	y-loc	zone				2F10.0, I10
3	Origin of Grid	x-loc	y-loc					2F10.0
4	Grid Cell Size	x-size	y-size					2F10.0
5	Grid Size	# x	# y	# z				3I10
6	Vertical Definition	# z low	# z up	ht surf layer	min cell ht low	min cell ht up		2I10, 3F10.0
7	Packet Terminator	END						10A1

Exhibit VI-2. REGION Packet Format

3. UNITS Packet Rules

The UNITS packet must be used whenever values for any species or implicit variable are input in other than internal units. Additionally, all user-defined variables must be named in this packet, even if they are already in internal units. When it appears, this packet should follow the REGION packet and precede all the others, since it can modify coordinates specified in other time-invariant packets.

Table VI-5 shows the internal units for all variables used by the SAI Airshed Model. Table VI-6 shows other standard units that can be used and the associated conversion factors for each variable. Table VI-7 shows the standard molecular weights for certain species. In addition to internal units or built-in standard units, the user can specify his own input units, conversion factors, and molecular weights. The following specific rules apply to this packet:

> If a species or an implicit variable is not defined in this packet, it is assumed to be already in the appropriate internal units.

> If the unit name for a variable is left blank, the program will provide space for that variable and no unit conversions will be performed.

> If the variable is in one of the standard alternate units shown in Table VI-6, the units should be named and the factor fields left blank; the built-in conversion factors will then be used.

> If the variable will be input in nonstandard units, the unit name should be nonblank and scaling factors provided; conversion will be made using the following formula:

$$var_{internal} = a*var_{input} + b \quad .$$

Table VI-5. Implicit Variable Names and Internal Units Used in the SAI Airshed Model

Variable Name	Internal Units	Code
Time	hr	*
HEIGHT	m	M
COORD	m	M
DIFFBREAK	m	M
REGIONTOP	m	M
ROUGHNESS	m	M
DIAMETER	m	M
SPEED	m/hr	M/HR
WINDX	m/hr	M/HR
WINDY	m/hr	M/HR
CARM	m/hr	M/HR
STACKVEL	m/hr	M/HR
FLOWRATE	m^3/hr	M3/HR
DIRECTION	radians (from N = 0)	RADN=0
TEMPERATUR	°K	DEGK
STACKTEMP	°K	DEGK
TGRADBELOW	°K/m	DEGK/M
TGRADABOVE	°K/m	DEGK/M
ATMOSPRESS	atm	ATMOSPHERE
EXPCLASS	unitless	*
VEGFACTOR	unitless	*
RADFACTOR	min^{-1}	*
Concentrations	ppm ($\mu g/m^3$ for AEROSOLS)	PPM MICROG/M3
CONCWATER	ppm	PPM
Point source emissions	g-mol/hr (g/hr for AEROSOLS)	GM/HR G/HR

---

* The units for these variables can not be changed by the UNITS packet.

Table VI-6. Standard Unit Conversions

Variable	Standard Units	Standard Unit Code	a*	b
TEMPERATUR	°K[†]	DEGK	-9.0	-9.0
	°C	DEGC	-9.0	273.15
	°F	DEGF	0.5555556	255.38
	°R	DEGR	0.5555556	-9.0
HEIGHT	m[†]	M	-9.0	-9.0
COORD	cm	CM	0.01	-9.0
ROUGHNESS	km	KM	1000.0	-9.0
DIFFBREAK	in	IN	0.0254	-9.0
REGIONTOP	ft	FT	0.3048	-9.0
DIAMETER	mi	MI	1609.344	-9.0
SPEED	m/hr[†]	M/HR	-9.0	-9.0
WINDX	km/hr	KM/HR	1000.0	-9.0
WINDY	mi/hr	MI/HR	1609.344	-9.0
CARM	m/min	M/MIN	60.0	-9.0
STACKVEL	ft/min	FT/MIN	18.288	-9.0
	m/sec	M/S	3600.0	-9.0
	ft/sec	FT/S	1097.28	-9.0
	knots	KNOTS	1852.0	-9.0
DIRECTION	radians (from N = 0)[†]	RADN=0	-9.0	-9.0
	radians (from S = 0)	RADS=0	-9.0	3.141593
	degrees (from N = 0)	DEGN=0	0.01745329	-9.0
	degrees (from S = 0)	DEGS=0	0.01745329	3.141593
	16-point (from S = 1)	16PTS=1	0.392699	2.748893
	16-point (from S = 16)	16PTS=16	0.392699	3.141593
	36-point (from S = 1)	36PTS=1	0.1745329	2.967059
	36-point (from S = 36)	36PTS=36	0.1745329	3.141593

Table VI-6 (Continued)

Variable	Standard Units	Standard Unit Code	a*	b
TGRADUPPER	°K/m†	DEGK/M	-9.0	-9.0
TGRADLOWER	°K/km	DEGK/KM	0.001	-9.0
	°C/m	DEGC/M	-9.0	-9.0
	°C/km	DEGC/KM	0.001	-9.0
	°F/ft	DEGF/FT	1.822689	-9.0
	°F/mi	DEGF/MI	0.0003452	-9.0
	°R/ft	DEGR/FT	1.822689	-9.0
	°R/mi	DEGR/MI	0.0003452	-9.0
ATMPRESS	atm†	ATMOSPHERE	-9.0	-9.0
	Bars	BARS	0.986923	-9.0
	mm of Hg	MMHG	0.0013158	-9.0
	ft of H_2O	FTH2O	0.029499	-9.0
	kg/cm^2	KG/CM2	0.967841	-9.0
	in of Hg	INHG	0.0334211	-9.0
	lb/in^2	LB/IN2	0.068046	-9.0
	psi	PSI	0.068046	-9.0
	millibars	MILLIBARS	0.0009869	-9.0
	in of H_2O	INH2O	0.0024582	-9.0
Concentrations	ppm†	PPM	-9.0	-9.0
CONCWATER	pptm	PPTM	0.1	-9.0
	pphm	PPHM	0.01	-9.0
	ppb	PPB	0.001	-9.0
	g mol/m^3	GM/M3	.24400	-9.0
	lb mol/ft^3	LBM/FT3	3.876x10"	-9.0
	μg/m^3	MICROG/M3	-0.0244	-9.0
	g/m^3	G/M3	-24400	-9.0
	lb/ft^3	LB/FT3	-3.876x10"	-9.0

Table VI-6 (Concluded)

Variable	Standard Units	Standard Unit Code	a*	b
Point Source emissions	g-mol/hr†	GM/HR	-9.0	-9.0
	g-mol/day	GM/D	0.0416667	-9.0
	lb-mol/hr	LBM/HR	453.592	-9.0
	lb-mol/day	LBM/D	18.89967	-9.0
	kg/hr	KG/HR	-1000.0	-9.0
	kg/day	KG/D	-41.6667	-9.0
	lb/hr	LB/HR	-453.592	-9.0
	lb/day	LB/D	-18.89967	-9.0
	ton/hr	TON/HR	-907184.0	-9.0
	ton/day	TON/D	-37799.3	-9.0
	ton/year	TON/YR	-103.6	-9.0

---

* When the multiplicative factor (a) is negative, but not -9., the molecular weight is used in the denominator, and the absolute value of a is used as the multiplier.

† Internal units.

Table VI-7. Standard Species Names and Molecular Weights Used for Unit Conversion

Species	Molecular Weight
NO	30.
NO2	46.
CO	28.
O3	48.
H2O2	34.
SO2	64.
HNO2	47.
H2O	18.
O2	32.
CO2	44.
SO4	96.
PAN	121.
PAR	16.
OLE	32.
ETH	32.
ARO	96.
AEROSOLS	1.
CH4	16.
TOTAL HC	16.
SOX	64.
NOX	46.
OXIDANT	48.

> If the variable is a species and the input values will be in mass units rather than mole units, the following formula will be used:

$$var_{internal} = (a*var_{input} + b)/mol\ wt \quad .$$

> If both a standard unit name and scaling factors are specified, a warning message will be printed and the user's scaling factors will be used.

> A designation of -9.0 indicates that the conversion factor is not to be applied.

> If the factor fields are not blank or zero, a molecular weight must be entered on the card. If the variable does not have a molecular weight, e.g., as in TEMPERATUR, either a -9.0 or a +1.0 should be entered in the molecular weight field.

The contents of each card in the UNITS packet are shown in Table VI-8 and the format is given in Exhibit VI-3.

Table VI-8. UNITS Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be UNITS, left adjusted
2 Unit Definition	Variable name 1-10	10A1	--	Can be a species name, implicit variable, user-defined variable, or either of two special names: > COORD--for station, point source, boundary, and vertical profile coordinates; > HEIGHT--for station height, point source, stack height, and vertical profile heights (note that this name does not apply to the height of the diffusion break or top of the region); conversions specified apply to values input in all subsequent packets
	Unit name 11-20	10A1	--	If field is left blank, no unit conversion will be performed; if this is one of the standard unit names listed in Table VI-6, the corresponding conversion factors will be used; if it is any other unit name, conversion factors must be input

Table VI-8 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
	Multiplicative factor (a) 21-30	F10.0	--	Can be left blank if standard conversion factors are to be used
	Additive factor (b) 31-40	F10.0	--	Can be left blank if standard conversions are to be used
	Molecular weight (c) 41-50	F10.0	--	Can be left blank if standard molecular weights are to be used; if the unit name does not belong to the standard set, this number should be set to 1., even for nonspecies variables
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number 1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	UNITS						60A1
2+	Unit Definition	var name	unit name	mult fact	add fact	molec wt		2(10A1), 3F10.0
3	Packet Terminator	END						10A1

Exhibit VI-3. UNITS Packet Format

4. STATIONS Packet Rules

The STATIONS packet must be included if the methods STATINTERP, POISSON, or DIVERGENCE are used for any variable. The STATIONS packet, if present, must appear before the first time interval; it must include all stations for which values may appear at any time within the span of the file. The number of station cards must not exceed the maximum number of stations specified in the CONTROL packet. Duplication of station names is considered an error resulting in termination of the run. The contents of each card in the STATIONS packet are shown in Table VI-9 and the format is given in Exhibit VI-4.

Table VI-9. STATIONS Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be STATIONS, left adjusted
2+ Station Name and Location				
	Station name 1-10	10A1	--	Can be any name except the same as that for another station, or blank, or ALL
	x-location 11-20	F10.0	m, unless COORD was specified in UNITS packet	x-coordinate of the station; this number must be specified
	y-location 21-30	F10.0	m, unless COORD was specified in UNITS packet	y-coordinate of the station; this number must be specified
	z- location 31-40	F10.0	m, unless HEIGHT was specified in UNITS packet	Height of the station above ground; if omitted, this number is assumed to be 0; for files that do not vary vertically, this number is ignored
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number 1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	STATIONS						60A1
2+	Station Name and Location	stn name	x-loc	y-loc	z-loc			10A1, 3F10.0
3	Packet Terminator	END						10A1

Exhibit VI-4. STATIONS Packet Format

5. POINT SOURCES Packet Rules

The POINT SOURCES packet is used for preparing the PTSOURCE file; it must appear before the first time interval and include all point sources for which values may appear at any time within the span of the file. There are two cards (a pair) required for each point source, and the number of pairs must equal the number of point sources specified on Card 4 of the CONTROL packet. Duplication of point source names is considered an error, resulting in termination of the run. The contents of each card in the POINT SOURCES packet are shown in Table VI-10 and the format is given in Exhibit VI-5.

Table VI-10. POINT SOURCES Packet for the PTSOURCE File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be POINT SOURCES, left adjusted
2+ Point Source Name and Location				
	Point source name 1-10	10A1	--	Can be any alphanumeric sequence except the same as that of another point source or type of source, or blank, or ALL
	Type 11-20	10A1	--	Can be any alphanumeric sequence except a point source name, or blank, or ALL; point sources of the same type are treated as a group when specifying the method for calculating emissions and when specifying the vertical method; they can also be treated as a group when specifying emissions or emission factors
	x-location 21-30	F10.1	m, unless COORD was specified in UNITS packet	x-coordinate of the point source with respect to the reference origin; this number must be specified
	y-location 31-40	F10.1	m, unless COORD was specified in UNITS packet	y-coordinate of the point source with respect to the reference origin; this number must be specified

Table VI-10 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
3+ Point Source Properties				
	Stack height 1-10	F10.0	m, unless HEIGHT was specified in UNITS packet	Height of the top of the stack above the ground; this number must be greater than zero
	Stack exit diameter* 11-20	F10.0	m, unless DIAMETER was specified in UNITS packet	Must be specified if it is to be used to calculate the flow rate for the PLUMERISE method
	Stack exit temperature 21-30	F10.0	°K, unless STACKTEMP was specified in UNITS packet	Used to calculate heat flux for the PLUMERISE method
	Stack exit velocity* 31-40	F10.0	m/hr, unless STACKVEL was specified in UNITS packet	Used with stack exit diameter to calculate flow rate for the PLUMERISE method
4 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

---

* If the vertical method PLUMERISE is to be used to calculate the height at which the emissions enter the modeling region, either both the stack exit diameter and stack exit velocity or the stack flow rate alone must be specified. Flow rate is specified in the EMISSIONS VALUES packet.

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	POINT SOURCES						60A1
2+	Point Source Name and Location	pt srce nam	type	x-loc	y-loc			2(10A1), 2F10.0
3+	Point Source Properties	stack ht	stack diam	stack temp	stack vel			4F10.0
4	Packet Terminator	END						10A1

Exhibit VI-5. POINT SOURCES Packet Format

6. BOUNDARIES Packet Rules

The BOUNDARIES packet, used for preparing the BOUNDARY file, must appear before the first time interval. It contains a set of line segments that define the boundary of the simulated area; each line segment is defined by two coordinate pairs that represent its end points. The line segments can appear in any order and, within each one, the end points can appear in any order, but the complete set must represent a closed figure (i.e., every end point must be identical to one, and only one, end point of another line segment). In addition, the figure represented must be nonconcave along each axis; that is, within a single row or column, any two cells within the simulated area must not have any nonsimulated cells between them.

The boundary line segments outline the edge cells within the inner area to be simulated. Figure VI-1 shows a 17 x 22 cell region in which the inner 15 x 20 area is to be simulated. In the figure, the boundary line segments are indicated by dotted lines. To ensure that the program succeeds in matching the end points of touching line segments, each end point should be defined to be in the center of the cell in which it lies. The number of boundary line segments input must not exceed the maximum number specified on Card 4 of the CONTROL packet. Duplication of line segment names is considered an error resulting in termination of the run.

The contents of each card in the BOUNDARIES packet are shown in Table VI-11 and the format is given in Exhibit VI-6.

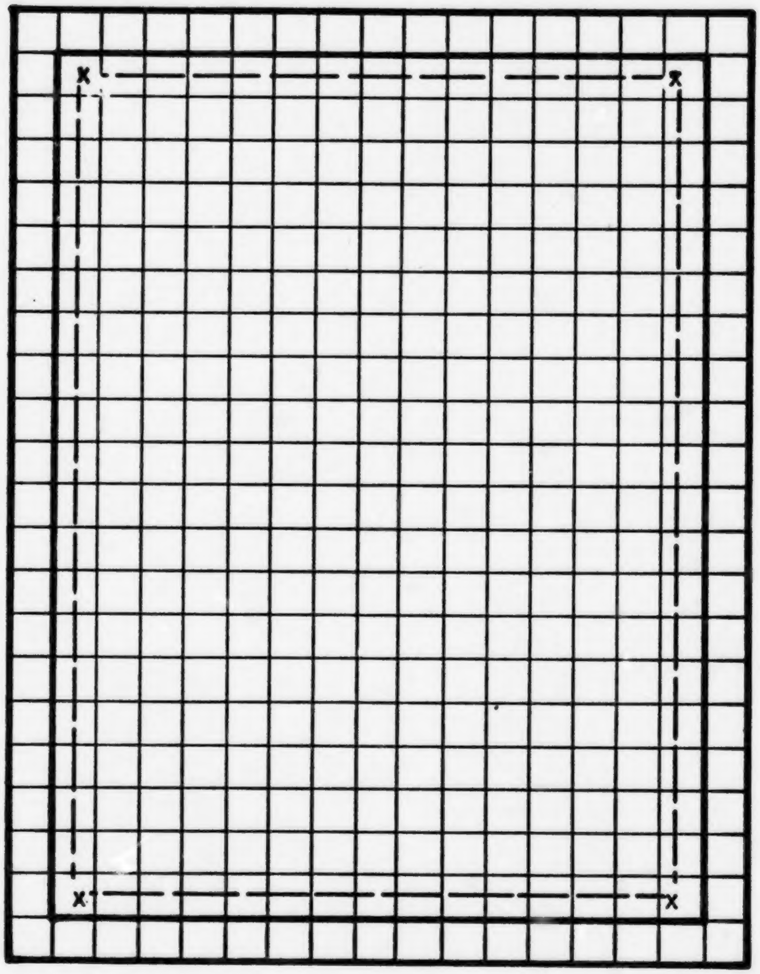


Figure VI-1. Definition of Boundary Line Segments

Table VI-11. BOUNDARIES Packet for the BOUNDARY File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be BOUNDARIES, left adjusted
2+ Boundary Definition				
	Line segment name 1-10	10A1	--	Any alphanumeric sequence except the same as that for another line segment name, blank, or ALL
	x-beginning 11-20	F10.0	m, unless COORD was specified in UNITS packet	x-coordinate of the first end point with respect to the reference origin; the end point should lie in the center of a cell
	y-beginning 21-30	F10.0	m, unless COORD was specified in UNITS packet	y-coordinate of the first end point with respect to the reference origin
	x-end 31-40	F10.0	m, unless COORD was specified in UNITS packet	x-coordinate of the second end point with respect to the reference origin
	y-end 41-50	F10.0	m, unless COORD was specified in UNITS packet	y-coordinate of the second end point with respect to the reference origin
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	BOUNDARIES						60A1
2+	Boundary Definition	line name	x-beg	y-beg	x-end	y-end		10A1, 4F10.0
3	Packet Terminator	END						10A1

Exhibit VI-6. BOUNDARIES Packet Format

7. TIME INTERVAL Packet Rules

A series of TIME INTERVAL packets follows the time-invariant data. The time intervals must be contiguous, must go forward, and must cover the entire time span of the file as specified in the CONTROL packet. If any time interval extends beyond the time span specified in the CONTROL packet, that time interval will be reset by the program to lie exactly within the time span of the file.

TIME INTERVAL packets contain other time-varying packets that define regional divisions, calculation methods, and time-varying data values. Each TIME INTERVAL packet consists of a header card, a time interval card, other packets as desired, and a terminator card. The contents of each card in the TIME INTERVAL packet is shown in Table VI-12 and the format is given in Exhibit VI-7. The other time-varying packets that can be included within the TIME INTERVAL packet for a given file are shown in the appropriate section of Chapter VII; their formats and rules are described in the remainder of this chapter.

Table VI-12. TIME INTERVAL Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be TIME INTERVAL, left adjusted
2 Time Interval	Beginning date 1-10	I10	Julian date (yyddd)	yy is the last two digits of the year and ddd is the three-digit Julian date
	Beginning time 11-20	I10	Military time (hhmm)	hh is hours and mm is minutes; this time will be internally converted to hours and fraction
	End date 21-30	I10	Julian date (yyddd)	Same format as beginning date
	End time 31-40	I10	Military time (hhmm)	Same format as beginning time
3 + Other Packets				Chapter VII lists the packets allowed here for each data file
4 Packet Terminator	Terminator 1-3	10A1	--	Must be ENDTIME, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	TIME INTERVAL						60A1
2	Time Interval	beg date	beg time	end date	end time			4I10
3+	Other Packets							
4	Packet Terminator	ENDTIME						10A1

Exhibit VI-7. TIME INTERVAL Packet Format

8. SUBREGION Packet Rules

The entire modeling region can be divided into subregions for data preparation purposes. Different data preparation methods or other parameters can be associated with each subregion. (These subregions should not be confused with "segments," which are divisions of the region for simulation purposes.) The subregion definitions may likely be different for the preparation of different types of data files; in fact, a subregion definition can be changed within the time span of a given file depending on the availability of or assumptions about the data.

A subregion name must be assigned to each grid square in the modeling region. The maximum number of subregion names that may be assigned is specified in the CONTROL packet. If this number = 1, the entire region is considered to be one subregion; nevertheless, the SUBREGION packet must be included and must appear at the beginning of the first TIME INTERVAL packet. In subsequent time intervals, the SUBREGION packet can be used to change subregion assignments. Only those portions of the region to be changed need be specified. New subregion names can be added provided that the maximum number allowed is not exceeded.

Subregion names are assigned by row. A typical subregion definition card contains a subregion name and a row in which it appears. For that row, a column number and cell count, n, are specified. Beginning at that column, the subregion name will be repeated for n columns along the row. The following conditions constitute errors resulting in termination of the program:

- > The cell count extends the column count beyond the edge of the region.
- > Any grid cell is unassigned.
- > The number of subregion names exceeds the maximum number specified in the CONTROL packet.

If the entire region is to be treated as one subregion, the SUBREGION packet should contain the following information:

```
SUBREGION
A---------|---------1|---------1|--------−1|
END       ,
```

where A (or some other simple name) is the subregion name. This name (or ALL) must then be used in the subregion field of all subsequent input cards.

The contents of each card in the SUBREGION packet are shown in Table VI-13 and the format is given in Exhibit VI-8.

Table VI-13. SUBREGION Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be SUBREGION, left adjusted
2+ Subregion Definition				
	Subregion name 1-10	10A1	--	Any alphanumeric sequence except blank or ALL
	Row number 11-20	I10	--	Must be ≥ 1, and $\leq$ number of rows (cells in y-direction) in region
	Beginning column number 21-30	I10	--	Must be ≥ 1, and $\leq$ number of columns (cells in x-direction) in region
	Cell count 31-40	I10	--	Must not exceed [(number of columns) - (column number) + 1]; if omitted, this value is assumed to be = rest of row; if negative, this value is assumed to be = rest of modeling region
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	SUBREGION						60A1
2+	Subregion Definition	subreg name	row #	beg col #	# cells			10A1, 3I10
3	Packet Terminator	END						10A1

Exhibit VI-8. SUBREGION Packet Format

9. METHOD Packet Rules

The METHOD packet is used to define the calculation method to be used for ground-level values of each variable in each subregion; it is required for all of the M.E.B. files except METSCALARS. The METHOD packet must appear in the first time interval, and it must directly follow the SUBREGION packet. In subsequent time intervals, the methods previously defined will persist unless they are respecified. If new subregions are defined in later time intervals, methods must also be defined for them. The contents of each card in the METHOD packet are shown in Table VI-14 and the format is given in Exhibit VI-9. Within the METHOD packet, each Method Definition card must be followed by its Parameter cards, if any. All of the calculation methods and the parameters required by each one are defined in Section VI.A.6. Chapter VII lists the particular methods that can be used for each file.

Table VI-14. METHOD Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be METHOD, left adjusted
2+ Method Definition				
	Subregion name 1-10	10A1	--	Must match a name in the subregion packet; if the name = ALL, this method will apply to this variable in all subregions
	Variable name 11-20	10A1	--	Must be an output species, implicit variable name, or user-defined variable name from the UNITS packet; if the variable name = ALL, this method will be used for all variables in this subregion
	Method 21-30	10A1	--	See Section VI.A.6 for standard method names
	Minimum value 31-40	F10.0	Internal units assumed, unless otherwise specified in UNITS packet	Lower bound for variable; if the variable name = ALL, this value will be converted according to unit specifications for the first variable; care should be taken in setting limits for ALL variables, especially when species (requiring different molecular weights for conversion) are involved; if the value calculated for the variable is less than this number, that value will be set equal to this number; if the field is left blank, it is assumed to be zero; if it is set to -9.0, no lower limit test will be performed

Table VI-14 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
	Maximum value 41-50	F10.0	Internal units assumed, unless otherwise specified in UNITS packet	Upper bound for variable; if the variable name = ALL, this value will be converted as described above; if the value calculated for this variable is greater than the number, that value will be set equal to this number; if the field is left blank, it is assumed to be zero; if it is set to -9.0, no upper limit test will be performed
	Number of parameters 51-60	I10	--	Defines the number of parameter cards that follow (Card 3 below); must be ≥ 0; Section VI.A.6 gives the number of parameters associated with each method
3+ Parameters				
	Parameter name 1-10	10A1	--	Standard parameter names and values are defined in Section VI.A.6; the number of parameter cards for a given method must equal the number specified on Card 2
	Parameter value 11-20	F10.0	--	
4 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	METHOD						60A1
2+	Method Definition	subreg name	var name	method	min value	max value	# params	3(10A1), 2F10.0, I10
3+	Parameters	param name	value					10A1,F10.0
4	Packet Terminator	END						10A1

Exhibit VI-9. METHOD Packet Format

10. VERTICAL METHOD Packet Rules

In general, where it is necessary to determine the values of variables in grid cells above ground level, a VERTICAL METHOD packet is required. The VERTICAL METHOD packet is used to define the calculation method to be used for obtaining values of each variable above ground level in each subregion. The VERTICAL METHOD packet must appear in the first time interval; it must follow the METHOD packet and precede the VERTICAL PROFILES packet (if any). In subsequent time intervals, the vertical methods previously defined will persist unless they are respecified. If new subregions are defined in later time intervals, vertical methods must also be defined for them. Within the VERTICAL METHOD packet, each vertical method definition card must be followed by its parameter cards, if any. All of the vertical calculation methods and the parameters required by each one are defined in Section VI.A.7. Chapter VII lists the particular vertical methods that can be used for each file. The contents of each card in the VERTICAL METHOD packet is shown in Table VI-15, and the format is given in Exhibit VI-10.

Table VI-15. VERTICAL METHOD Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be VERTICAL METHOD, left adjusted
2+ Vertical Method Definition				
	Subregion name 1-10	10A1	--	Must match a name in the subregion packet; if the name = ALL, this vertical method will apply to this variable in all subregions
	Variable name 11-20	10A1	--	Must be an output species, implicit variable name, or user-defined variable name from the UNITS packet; if the variable name = ALL, this vertical method will be used for all variables in this subregion
	Method 21-30	10A1	--	See Section VI.A.7 for standard vertical method names
	Minimum value 31-40	F10.0	Internal units, unless otherwise specified in UNITS packet	Lower bound for variable; as in the METHOD packet, if the variable name = ALL, this value will be converted according to unit specifications for the first variable; if the value calculated for the variable is less than this number, that value will be set equal to this number; if the field is left blank, it is assumed to be zero; if it is set to -9.0, no lower limit test will be performed

Table VI-15 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
	Maximum value 41-50	F10.0	Internal units, unless otherwise specified in UNITS packet	Upper bound for variable; if the variable name = ALL, this value will be converted as described above; if the value calculated for this variable is greater than this number, that value will be set equal to this number; if the field is left blank, it is assumed to be zero; if it is set to -9.0, no upper limit test will be performed
	Number of parameters 51-60	I10	--	Defines the number of parameter cards that follow (Card 3 below); must be≥ 0; Section VI.A.7 gives the number of parameters associated with each vertical method
3+ Parameters				Standard parameter names and values are defined in Section VI.A.7; the number of parameter cards for a given vertical method must equal the number specified on Card 2
	Parameter name 1-10	10A1	--	
	Parameter value 11-21	F10.0	--	
4 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	VERTICAL METHOD						60A1
2+	Vertical Method Definition	subreg name	var name	method	min value	max value	# param	3(10A1), 2F10.0 I10
3+	Parameters	param name	value					10A1, F10.0
4	Packet Terminator	END						10A1

Exhibit VI-10. VERTICAL METHOD Packet Format

11. CONSTANTS Packet Rules

The CONSTANTS packet is required in the first time interval if the method for any variable in any subregion has been specified as CONSTANT. All constant values can be included in one packet or, if desired, they can be grouped in several packets. In either case, all constant values must be specified in the initial time interval and will persist in subsequent time intervals unless they are explicitly changed. The contents of each card in the CONSTANTS packet are shown in Table VI-16 and the format is given in Exhibit VI-11.

Table VI-16. CONSTANTS Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be CONSTANTS, left adjusted
2+ Constants				
	Subregion name 1-10	10A1	--	Must be identical to a previously named subregion, or ALL; if ALL is specified, all subregions that use the CONSTANT method for this variable will be assigned this value
	Variable name 11-20	10A1	--	Must be a variable named on a method card that specifies CONSTANT; if ALL is specified, all variables that require CONSTANT for this subregion will be assigned this value
	Value 21-30	F10.0	Internal units, unless otherwise specified in UNITS packet	If the variable name = ALL, this value will be converted according to unit specifications for the first variable; care should be taken in specifying values for ALL variables, especially when species (requiring different molecular weights for conversion) are involved
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	CONSTANTS						60A1
2+	Constants	subreg name	var name	value				2(10A1), F10.0
3	Packet Terminator	END						10A1

Exhibit VI-11. CONSTANTS Packet Format

12. GRID VALUES Packet Rules

The GRID VALUES packet must be included in the first time interval if the method for any variable in any subregion has been specified as GRID VALUE. All grid values can be included in one packet or, if desired, they can be grouped in several packets. In either case, all grid values must be specified in the initial time interval and will persist in subsequent time intervals unless they are explicitly changed. The contents of each card in the GRID VALUES packet are shown in Table VI-17 and the format is shown in Exhibit VI-12.

Table VI-17. GRID VALUES Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be GRID VALUES, left adjusted
2+ Grid Values				
	Subregion name 1-10	10A1	--	Must be identical to a previously named subregion; GRID VALUES must be specified as the method for this variable
	Variable name 11-20	10A1	--	Must be a variable named or implied (by means of ALL) on a method card for this subregion
	Column number 21-30	I10	--	y-index on grid, counting from bottom (SOUTH) row = 1
	Row number 31-40	I10	--	x-index on grid, counting from left (WEST) column = 1
	Value 41-50	F10.0	Internal units, unless otherwise specified in UNITS packet	If the variable name = ALL, this value will be converted according to unit specifications for the first variables; care should be taken in specifying values for ALL variables especially when species (requiring different molecular weights for conversion) are involved.
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	GRID VALUES						60A1
2+	Grid Values	subreg name	var name	col #	row #	value		2(10A1), 2I10, F10.0
3	Packet Terminator	END						10A1

Exhibit VI-12. GRID VALUES Packet Format

13. STATION READINGS Packet Rules

The STATION READINGS packet must appear in the first time interval when the method for any variable in any subregion has been specified as STATINTERP, POISSON, or DIVERGENCE. A value that does not appear in the first time interval for a station-variable pair is recognized as "missing", and the station will not be included in the calculation. In subsequent time intervals, the STATION READINGS packet can be used to modify existing data in the following ways:

- An existing reading can be changed by substituting a new value.
- An existing reading can be nullified (i.e., changed to "missing") by supplying a value of -9.0.
- A "missing" reading can be changed to "nonmissing" by supplying a value.

For any station-variable pair not supplied, the previous values, "missing" or not, will persist. The contents of each card in the STATION READINGS packet is shown in Table VI-18 and the format is given in Exhibit VI-13.

Table VI-18. STATION READINGS Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be STATION READINGS, left adjusted
2+ Station Readings				
	Station name 1-10	10A1	--	Must be identical to a name specified in the STATIONS packet
	Variable name 11-20	10A1	--	Must be a species name, or an implicit or user-defined variable
	Value 21-30	F10.0	Internal units, unless otherwise specified	A blank is treated as zero; -9.0 is considered "missing"
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number 1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	STATION READINGS						60A1
2	Station Readings	stn name	var name	value				2(10A1), F10.0
3	Packet Terminator	END						10A1

Exhibit VI-13. STATION READINGS Packet Format

14. EMISSIONS VALUES Packet Rules

The EMISSIONS VALUES packet is used to create the PTSOURCE file. It provides emissions values for those variables for which the method EMVALUES was specified. The EMISSIONS VALUES packet must be included in the first time interval (unless all emissions are zero); any value not appearing in the first time interval for a point source-species pair will be assumed to be zero. In subsequent time intervals, existing data will persist unless explicitly changed. If all point sources of a given type have the same emissions values, the type can be specified instead of individual point source names.

If the vertical method PLUMERISE has been specified for a point source type, the variable FLOWRATE must be either input in the EMISSIONS VALUES packet or calculated. If it is not input, it will be calculated from the stack diameter and exit velocity input in the POINT SOURCES packet.

The contents of each card in the EMISSIONS VALUES packet are shown in Table VI-19 and the format is given in Exhibit VI-14.

Table VI-19. EMISSIONS VALUES Packet for the PTSOURCE File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be EMISSIONS VALUES, left adjusted
2+ Point Source Emissions				
	Point source or type 1-10	10A1	--	Must be one of the following: > a name appearing in the POINT SOURCES packet, > ALL--meaning all point sources, > a type appearing in the POINT SOURCES packet, meaning all point sources of a given type
	Variable name 11-20	10A1	--	Must be an output species or a user-defined input variable, or FLOWRATE
	Value 21-30	F10.0	gm-mol/hr (gm/hr for AEROSOLS), unless otherwise specified in UNITS packet	Emissions of the variable from the point source; if the variable is FLOWRATE, the units are m^3/hr, unless otherwise specified in the UNITS packet
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number 1-10	 11-20	 21-30	 31-40	 41-50	 51-60	FORTRAN Format
1	Packet Header	EMISSIONS VALUES						60A1
2+	Point Source Emissions	pt srce or type	var name	value				2(10A1), F10.0
3	Packet Terminator	END						10A1

Exhibit VI-14. EMISSIONS VALUES Packet Format

15. EMISSIONS FACTORS Packet Rules

The EMISSIONS FACTORS packet can be input for a given time interval to scale the emissions values previously input. The factors are used only if the method EMFACTORS was specified for the variable and point source type. The following formula will be used:

$$\text{output emissions (source, species)} = \text{factor (source, species)} \times \text{emissions (source, species)} \quad .$$

The factor is always applied to the last emissions value input in an EMISSIONS VALUES packet, not the last one calculated by a previous emissions factor. If factors are not input, they are assumed to be 1.0 (or the previous value specified). Emissions factors are applied to numbers in internal units--they are thus to be used to describe temporal variation rather than unit conversion. The contents of each card in the EMISSIONS FACTORS packet are shown in Table VI-20 and the format is given in Exhibit VI-15.

Table VI-20. EMISSIONS FACTORS Packet for the PTSOURCE File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be EMISSIONS FACTORS, left adjusted
2+ Emissions Factors	Point source or type 1-10	10A1	--	Must be one of the following: > a name appearing in the POINT SOURCES packet, > ALL--meaning all point sources, > a type appearing in the POINT SOURCES packet, meaning all point sources of a given type
	Variable name 11-20	10A1	--	Must be an output species or a user-defined input variable; if the name = ALL, this factor will apply to all species and to FLOWRATE
	Factor 21-30	F10.0	--	Emission factors apply to FLOWRATE as well as to species; when the variable = ALL, these factors are automatically applied; when factors are being provided for individual species, the factor for the flow rate, if it changes, must also be specified
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	EMISSIONS	FACTORS					60A1
2+	Emissions Factors	pt srce or type	var name	factor				2(10A1), F10.0
3	Packet Terminator	END						10A1

Exhibit VI-15. EMISSIONS FACTORS Packet Format

16. BOUNDARY READINGS Packet Rules

The BOUNDARY READINGS packet is used to create the BOUNDARY file; it provides values for those variables for which the method BOUNDVALUE was specified. The packet must be input for the first time interval. Concentration values at ground level are specified for each species for each boundary line segment; missing values are considered an error. In subsequent time intervals, only the data to be changed need be specified. The contents of each card in the BOUNDARY READINGS packet is shown in Table VI-21, and the format is given in Exhibit VI-16.

Table VI-21. BOUNDARY READINGS Packet for the BOUNDARY File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be BOUNDARY READINGS, leftadjusted
2+ Boundary Values				
	Line segment name 1-10	10A1	--	Must be a name specified in the BOUNDARY packet, or ALL
	Variable name 11-20	10A1	--	Must be an output species, a user-defined variable, or ALL
	Value 21-30	F10.0	ppm (μg/m^3 for AEROSOLS), unless otherwise specified in UNITS packet	Ground-level concentration of the variable along the line segment
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	BOUNDARY READINGS						60A1
2+	Boundary Values	line name	var name	value				2(10A1), F10.0
3	Packet Terminator	END						10A1

Exhibit VI-16. BOUNDARY READINGS Packet Format

17. SCALARS Packet Rules

The SCALARS packet must be input for the first time interval for the METSCALARS file. For this time interval, all six meteorological scalars (TGRADBELOW, TGRADABOVE, EXPCLASS, RADFACTOR, CONCWATER, and ATMOSPRESS) must be assigned values. Missing values are considered errors. In subsequent time intervals, only the data to be changed need be specified. The contents of each card in the SCALARS packet is shown in Table VI-22 and the format is given in Exhibit VI-17.

Table VI-22. SCALARS Packet for the METSCALARS File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be SCALARS, left adjusted
2+ Meteorological Scalars				
	Scalar name 1-10	10A1	--	Must match the standard spelling of the scalars (see Chapter VII for instructions on preparing the METSCALARS file)
	Value 11-20	F10.0	Internal units, unless otherwise specified in UNITS packet	
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	SCALARS						60A1
2+	Scalars	scalar name	value					10A1, F10.0
3	Packet Terminator	END						10A1

Exhibit VI-17. SCALARS Packet Format

18. VERTICAL PROFILES Packet Rules

For some vertical methods, a profile is required (see Section VI.A.7 for details). The VERTICAL PROFILES packet must contain a profile for each subregion-variable pair requiring one. Each profile must contain at least two points, which must be entered in order of increasing height. The first point always represents ground level. There can be only one vertical profile specified for a given subregion and variable. Each profile consists of a description card followed by a set of height/value pairs. The contents of each card in the VERTICAL PROFILES packet is shown in Table VI-23 and the format is given in Exhibit VI-18.

Table VI-23. VERTICAL PROFILES Packet for M.E.B. Files

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be VERTICAL PROFILES, left adjusted
2+ Profile Description				
	Subregion name 1-10	10A1	--	Must be identical to a previously named subregion, or boundary line segment, or ALL; if ALL is specified, all subregions that require a vertical profile for this variable will use these values
	Variable name 11-20	10A1	--	Must be a variable that requires a vertical profile for this subregion; if name = ALL, this profile will be used for all variables in this subregion
	x-location 21-30	F10.0	m, unless COORD was specified in UNITS packet	x-coordinate of the profile with respect to the reference origin; this number will be ignored if a "relative" method is not being used
	y-location 31-40	F10.0	m, unless COORD was specified in UNITS packet	y-coordinate of the profile with respect to the reference origin; this number will be ignored if a "relative" method is not being used
	Number of points 41-50	I10	--	Number of profile points that follow; must be ≥ 2 (or = -9 to clear all profile points)

Table VI-23 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
3+ Profile Points				
	Height 1-10	F10.0	m, unless HEIGHT was specified in UNITS packet	Must be in increasing order; the first is assumed to be ground level and will be subtracted from all others to obtain each height relative to the ground
	Value 11-20	F10.0	--	See the appropriate vertical method description in Section VI.A.7
4 Packet Terminator	Terminator	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	VERTICAL PROFILES						60A1
2+	Profile Description	subreg name	var name	x-loc	y-loc	# pts		2(10A1), 2F10.0, I10
3+	Profile	height	value					2F10.0
4	Packet Terminator	END						10A1

Exhibit VI-18. VERTICAL PROFILES Packet Rules

VII M.E.B. FILE PREPARATION RULES AND EXAMPLES

Chapter VI presented the data preparation packets--the building blocks used to generate the M.E.B. data files. This chapter presents detailed instructions for the creation of each file, using the packets described above.

The preparation of some data files may require that other files be input, depending on the method used. In general, vertically varying files may require information from DIFFBREAK and REGIONTOP to define the vertical distribution of grid cells. The following is a suggested order of file preparation, assuming methods requiring the greatest file dependency. This order may be varied, depending on the requirements of the actual methods used.

> DIFFBREAK.
> EMISSIONS.
> METSCALARS.
> TEMPERATUR.
> TERRAIN.
> REGIONTOP (requiring DIFFBREAK).
> TOPCONC (requiring DIFFBREAK and REGIONTOP).
> AIRQUALITY (requiring DIFFBREAK, REGIONTOP, and TOPCONC).
> BOUNDARY (requiring DIFFBREAK, REGIONTOP, and TOPCONC).
> WIND (requiring DIFFBREAK, REGIONTOP, and TEMPERATUR).
> PTSOURCE (requiring DIFFBREAK, REGIONTOP, METSCALARS, TEMPERATUR, and WIND).

The output from each program can include a printout of the input a title page, tables of methods, vertical methods, vertical profiles, a subregion grid, and grids of output variable values. In this manual, a sample of each type of output is shown only for the AIRQUALITY file (Exhibit VII-2). For the other M.E.B. files, only the title page, methods tables, and an output grid sample are shown.

The data file preparation instructions are presented alphabetically by file name; each section includes:

- > A short description of the file.
- > The variables required and their units.
- > The computation methods that can be used.
- > The time variation represented.
- > The arrangement of packets in the input deck and special instructions for each one.
- > Additional input files required.
- > Sample input and output from a file generation run.

A. AIRQUALITY

The AIRQUALITY file contains a three-dimensional matrix of concentrations for any number of chemical species. Its primary purpose is to provide the set of initial conditions for the beginning of the modeling period; however, it can also be used to prepare a three-dimensional distribution of measured data in any time interval for use in comparison studies. The program AIRQUL is used to create the AIRQUALITY file. AIRQUL requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-1 is an information flow diagram illustrating the job control to be used. The following sections discuss the input to the AIRQUL program.

1. Variables

The output variables for the AIRQUALITY file are the species named in the CONTROL packet. Additional user-defined input variables (e.g., "reactive hydrocarbons") can be specified in the UNITS packet. The internal units for the concentrations of all species except AEROSOLS are parts per million (ppm); for AEROSOLS, the units are micrograms per cubic meter ($\mu g/m^3$). The standard names for reactive species currently recognized by the Airshed Simulation Program are listed in Section IX.A. If any of these species does not appear on the AIRQUALITY file, the initial concentrations will default to a value defined in the CHEMPARAM file. If any additional species appear on AIRQUALITY, they will be ignored.

2. Methods

The methods that can be used to generate the AIRQUALITY file are:

> CONSTANT
> GRID VALUE
> STATINTERP
> POISSON

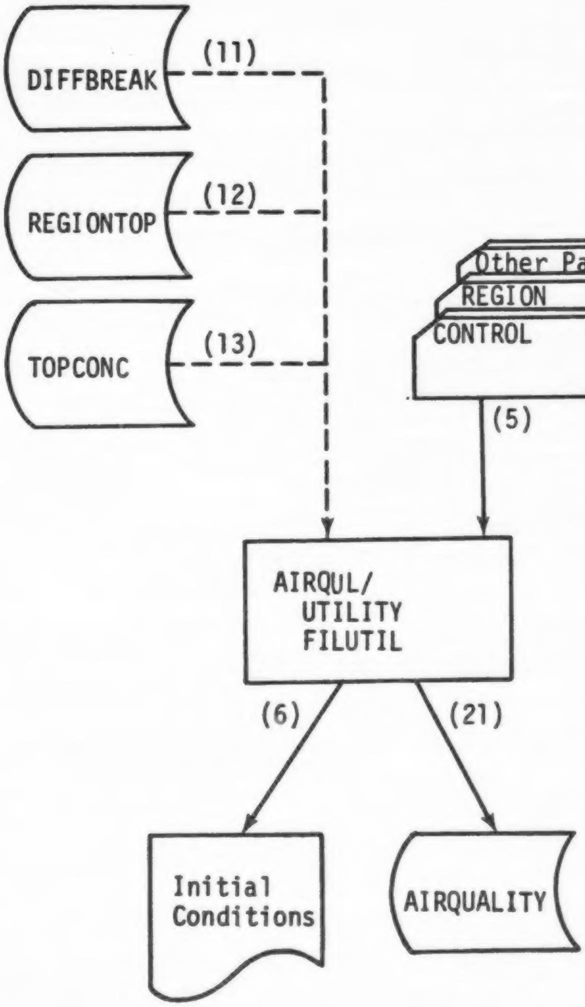

DIFFBREAK
(11)
REGIONTOP
(12)
TOPCONC
(13)
Other Packets
REGION
CONTROL
(5)
AIRQUL/
UTILITY
FILUTIL
(6)
(21)
Initial
Conditions
AIRQUALITY

Figure VII-1. Information Flow Diagram for the AIRQUALITY File

> SPLIT/COMB
> E-WINTERP
> N-SINTERP
> USER.

These methods are discussed in detail in Section VI.A.6.

Since the AIRQUALITY file varies in the vertical direction, a vertical method must also be specified for each output variable in each subregion. The vertical methods that can be used are:

> CONSTANT
> ABSPROFILE
> RELPROFILE
> ABSPROFRAT
> RELPROFRAT
> E-WINTERP
> N-SINTERP
> VERTUSER.

These vertical methods are discussed in detail in Section VI.A.7.

3. Time Variation

The concentrations on the AIRQUALITY file are used as initial conditions for the Airshed Simulation Program. The time span of the file must therefore include the beginning simulation time. Furthermore, the time interval containing the data to be used must begin at or before the simulation starting time and must end after the simulation starting time. In the example in Exhibit VII-1 in this chapter, the time interval for the initial concentrations is 0500 to 0501.

4. Packets

Figure VII-2 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the file:

> CONTROL
- The file name on Card 2 must be AIRQUALITY.
- The control variables to be specified on Cards 4 to 8 for AIRQUALITY are shown in Table VII-1.
- The number of species must be greater than zero.
- If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named.
- If data from measuring stations are to be used (methods STATINTERP or POISSON), the maximum number of such stations must be given.
- The number of subregions must be at least one.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) must include maximum vertical parameter and profile entries as applicable.
- The file unit assignment card (No. 8) must provide entries for the DIFFBREAK, REGIONTOP, and TOPCONC files if, and only if, these files are required by the vertical methods selected.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is required; their number must be the same as the entry in the first control parameter on Card 4. If either the ABSPROFRAT or RELPROFRAT vertical method is selected for any variable, the output species names specified here must match the species names on the TOPCONC file.

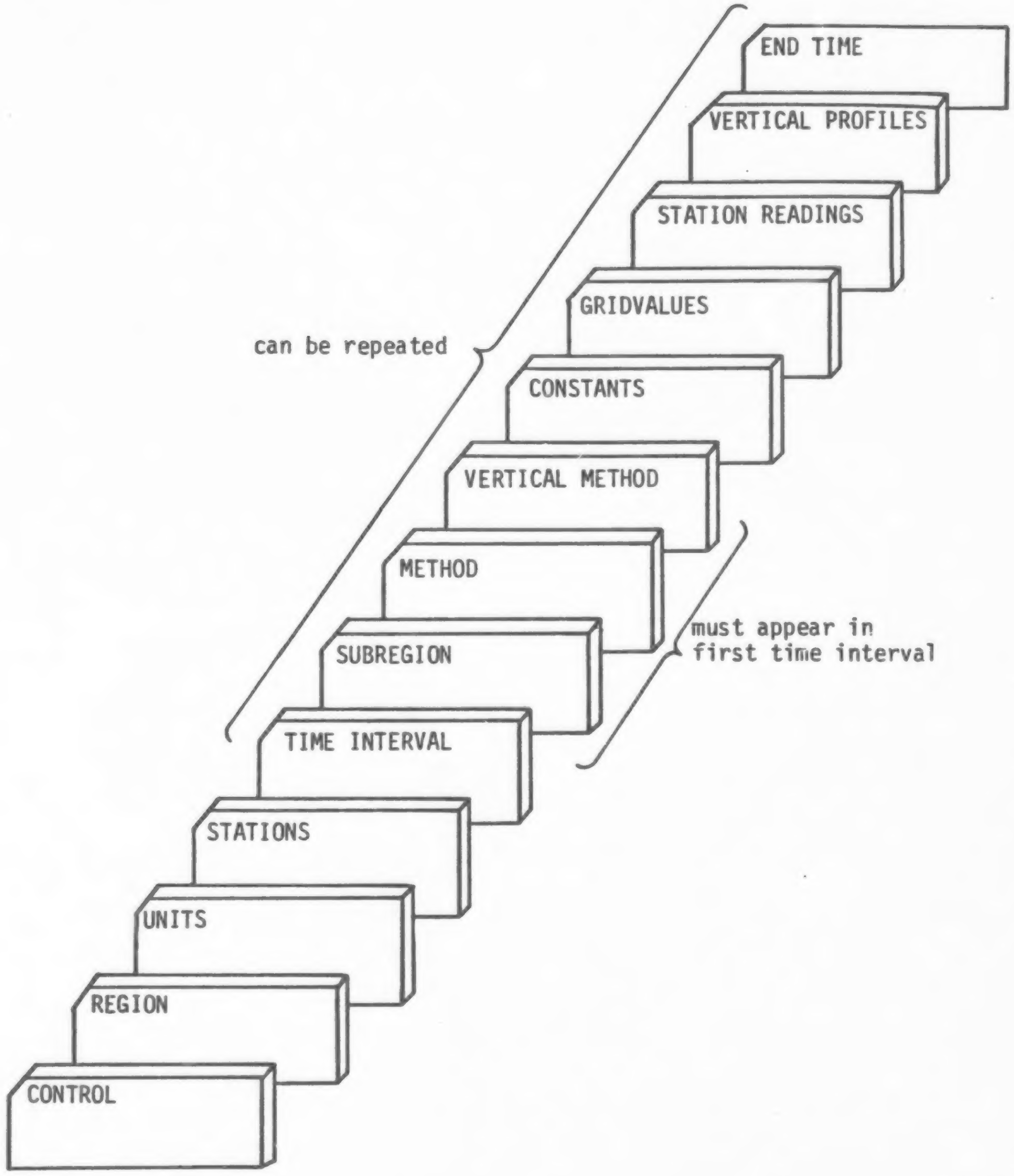

END TIME
VERTICAL PROFILES
STATION READINGS
GRIDVALUES
can be repeated
CONSTANTS
VERTICAL METHOD
METHOD
must appear in first time interval
SUBREGION
TIME INTERVAL
STATIONS
UNITS
REGION
CONTROL

Figure VII-2. Input Card Deck Structure for Preparing the AIRQUALITY File

Table VII-1. CONTROL Packet Entries for the AIRQUALITY File

Card Number	Entry
4	Number of species
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Number of vertical parameters
	Number of heights in profile
	Print vertical methods table
	Print vertical profile tables
	Spare
	Spare
8	DIFFBREAK file number
	REGIONTOP file number
	TOPCONC file number
	Spare
	Spare
	Spare

> REGION. This packet must follow the CONTROL packet. The vertical parameters must be provided for the AIRQUALITY file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:
>
> - Any input variable will be input in other than internal units.
> - Any user-defined variables are specified.
> - COORD or HEIGHT unit conversions are to be used.
>
> The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> STATIONS. This packet is required if either of the methods STATINTERP or POISSON is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.

> TIME INTERVAL. One or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> SUBREGION. The first time interval must contain a SUBREGION packet; the inclusion of this packet in other time intervals is optional. The number of subregions must not exceed the maximum specified in the CONTROL packet.

> METHOD. A method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> VERTICAL METHOD. A vertical method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Vertical methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each vertical parameter entry contributes to the overall vertical parameter count; the total must not exceed the maximum specified in the CONTROL packet.

> CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.

> GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, the first time interval must contain a GRID VALUES packet. More than one GRID VALUES packet can appear in any time interval.

> STATION READINGS. If either the POISSON or STATINTERP method is assigned to any species in the METHOD packet, the first time interval must contain a STATION READINGS packet. More than one STATION READINGS packet can appear in any time interval.

> VERTICAL PROFILES. If any of the profile methods are assigned to any species in the VERTICAL METHOD packet, the first time interval must contain a VERTICAL PROFILES packet. There must be a vertical profile defined (or implied using ALL) for every variable in every subregion for which a profile method was specified. The number of height-value pairs in any single profile must not exceed the maximum specified in the CONTROL packet. More than one VERTICAL PROFILES packet can appear in any time interval.

5. Additional Input Files

If any vertical method besides CONSTANT was selected, the DIFFBREAK and REGIONTOP files must be input to AIRQUL. In addition, if either of the vertical methods ABSPROFRAT or RELPROFRAT was selected, the TOPCONC file must also be input.

6. Examples

Exhibit VII-1 shows a sample input deck for AIRQUALITY file generation. The output from an AIRQUL run using that input deck is shown in Exhibit VII-2.

```
CONTRUL
AIR QUALITY
 INITIAL POLLUTANT CONCENTRATIONS  ST LOUIS  500  76195
        11         1        25         1        30         5
        21         1         1
                                       1
         5         5         1         0
        11        12        13
NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
     76195       500     76195       501
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.      50.0      200.
END
```

Exhibit VII-1.   Sample Input Deck for the AIRQUL Program

```
STATIONS
       101    19183.    27862.       10.
       102    17518.    34045.       10.
       103    22588.    30467.       10.
       104    22312.    25304.       10.
       105    18706.    24453.       10.
       106    13660.    25566.       10.
       107    15179.    30610.       10.
       108    23407.    39102.       10.
       109    30802.    27886.       10.
       110    22209.    20826.       10.
       111    13812.    20479.       10.
       112     8938.    28913.       10.
       113    12738.    37820.       10.
       114    19320.    45456.       10.
       115    32111.    45799.       10.
       116    37777.    38083.       10.
       117    35560.    20818.       10.
       118    18065.    11256.       10.
       119     4759.    18547.       10.
       120    -1921.    33909.       10.
       121     7414.    50376.       10.
       122    16631.    77223.       10.
       123    52320.    34378.       10.
       124    24275.   -15463.       10.




       125   -27555.    30240.       10.
END
TIME INTERVAL·
    76195        500     76195       501
SUBREGION
A                  1         1        -1
END
```

Exhibit VII-1 (Continued)

```
METHOD
A         NO        POISSON      .00100     1.00        3
MAXITER        100
ERRORTOL  .001000
OMEGA          1.4
A         NO2       POISSON      .00100     1.00        3
MAXITER        100
ERRORTOL  .001000
OMEGA          1.4
A         O3        POISSON      .00100     1.00        3
MAXITER        100
ERRORTOL  .001000
OMEGA          1.4
A         RHC       POISSON      .05000     4.00        3
MAXITER        100
ERRORTOL  .050000
OMEGA          1.4
A         ETH       SPLIT/COMB   .00100     4.00        1
RHC          .0217
A         OLE       SPLIT/COMB   .00100     4.00        1
RHC          .0440
A         PAR       SPLIT/COMB   .01000     4.00        1
RHC          .6665
A         CARB      SPLIT/COMB   .00100     4.00        1
RHC          .0810
A         ARO       SPLIT/COMB   .00010     4.00        1
RHC          .0248
A         BZA       SPLIT/COMB   .00000     4.00        1
RHC          .0001
A         PAN       CONSTANT     .00001      .10        0
A         CO        POISSON      .10000    20.00        3
MAXITER        100 .
ERRORTOL  .100000
OMEGA          1.4
END
VERTICAL METHOD
ALL       ALL       RELPROFRAT   .0000     100.0
END
CONSTANTS
A         PAN          .000010
END
```

Exhibit VII-1 (Continued)

```
STATION READINGS                                            INITIAL COND  500
  101       03            .024
  102       03          -9.000
  103       03            .027
  104       03          -9.000
  105       03            .002
  106       03            .022
  107       03            .030
  108       03            .027
  109       03            .038
  110       03            .035
  111       03          -9.000
  112       03            .028
  113       03            .034
  114       03            .036
  115       03          -9.000
  116       03            .035
  117       03            .036
  118       03          -9.000
  119       03            .029
  120       03            .019
  121       03            .002
  122       03            .043
  123       03          -9.000
  124       03            .024
  125       03            .003
  101       CO            .254
  102       CO            .050
  103       CO            .174
  104       CO          -9.000
  105       CO            .050
  106       CO            .185
  107       CO            .226
  108       CO            .055
  109       CO            .050
  110       CO          -9.000
  111       CO            .059
  112       CO            .267
  113       CO            .209
  114       CO            .109
  115       CO            .050
  116       CO          -9.000
  117       CO            .148
  118       CO            .050
  119       CO            .320
  120       CO            .239
  121       CO            .108
  122       CO            .050
```

Exhibit VII-1 (Continued)

```
123    CO          .175
124    CO          .256
125    CO          .077
101    RHC       -9.000
102    RHC         .131
103    RHC         .086
104    RHC         .178
105    RHC       -9.000
106    RHC         .196
107    RHC         .146
108    RHC         .060
109    RHC       -9.000
110    RHC       -9.000
111    RHC         .082
112    RHC         .117
113    RHC         .050
114    RHC       -9.000
115    RHC       -9.000
116    RHC       -9.000
117    RHC       -9.000
118    RHC       -9.000
119    RHC         .050
120    RHC         .474
121    RHC       -9.000
122    RHC       -9.000
123    RHC       -9.000
124    RHC       -9.000
125    RHC       -9.000
101    NO          .002
102    NO          .002
103    NO          .003
104    NO          .002
105    NO        -9.000
106    NO          .002
107    NO          .003
108    NO          .005
109    NO          .002
110    NO          .002
111    NO          .002
112    NO          .002
113    NO          .003
114    NO          .002
115    NO          .002
116    NO          .002
117    NO          .002
```

Exhibit VII-1 (Continued)

```
118      NO            .002
119      NO            .002
120      NO            .003
121      NO            .002
122      NO            .002
123      NO            .002
124      NO            .002
125      NO            .002
101      NO2           .020
102      NO2           .004
103      NO2           .010
104      NO2         -9.000
105      NO2         -9.000
106      NO2           .002
107      NO2           .011
108      NO2           .010
109      NO2           .002
110      NO2           .005
111      NO2           .018
112      NO2           .016
113      NO2           .010
114      NO2           .008
115      NO2           .002
116      NO2           .002
117      NO2           .002
118      NO2           .003
119      NO2           .011
120      NO2           .022
121      NO2           .005
122      NO2           .002
123      NO2           .002
124      NO2           .003
125      NO2           .002
END
VERTICAL PROFILE
A          ALL         35296.     5038.        4
       0.         0.
     100.         0.
     120.         1.
     500.         1.
END
ENDTIME
```

Exhibit VII-1 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE AIRQUALITY
 INITIAL POLLUTANT CONCENTRATIONS  ST LOUIS  500  76195

NUMBER OF USER-DEFINED VARIABLES =          1
NUMBER OF STATIONS =         25
NUMBER OF SUBREGIONS =          1
NUMBER OF METHOD PARAMETERS =          30
NUMBER OF VERTICAL METHOD PARAMETERS =          5
NUMBER OF VERTICAL PROFILE HEIGHTS =          5
PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER         21
INPUT DATA FOR DIFFUSION BREAK WILL BE OBTAINED FROM FILE NUMBER         11
INPUT DATA FOR REGION TOP WILL BE OBTAINED FROM FILE NUMBER         12
INPUT DATA FOR TOP CONCENTRATIONS WILL BE OBTAINED FROM FILE NUMBER         13
INPUT CARDS WILL BE PRINTED
OUTPUT GRID WILL BE PRINTED
UNIT TABLE WILL NOT BE PRINTED
STATION LOCATIONS WILL NOT BE PRINTED
SUBREGION GRID WILL NOT BE PRINTED
METHOD TABLE WILL BE PRINTED
STATION VALUES WILL NOT BE PRINTED
VERTICAL METHOD TABLE WILL BE PRINTED
VERTICAL PROFILE VALUES WILL NOT BE PRINTED
BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       5.00
ENDING DATE OF FILE      76195 ENDING TIME OF FILE       5.02
```

Exhibit VII-2.   Sample Output From the AIRQUL Program

```
A TOTAL OF         11 SPECIES NAMES WERE READ, THE SPECIES NAMES ARE --

NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
REGION
   723000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
```

Exhibit VII-2 (Continued)

```
                                         REGIONAL DEFINITION

UTM ORIGIN X-COORDINATE                       725000.

UTM ORIGIN Y-COORDINATE                      4252000.

UTM ORIGIN ZONE NUMBER                             15

REGION ORIGIN X-COORDINATE                    -19000.

REGION ORIGIN Y-COORDINATE                    -16000.

CELL LENGTH IN X-DIRECTION                    4000.00

CELL LENGTH IN Y-DIRECTION                    4000.00

NUMBER OF CELLS IN X-DIRECTION                     17

NUMBER OF CELLS IN Y-DIRECTION                     22

NUMBER OF CELLS IN Z-DIRECTION                      4

NUMBER OF CELLS IN LOWER VERTICAL LAYER             2

NUMBER OF CELLS IN UPPER VERTICAL LAYER             2

HEIGHT OF SURFACE LAYER                           .00

MINIMUM CELL HEIGHT IN LOWER LAYER              50.00

MINIMUM CELL HEIGHT IN UPPER LAYER             200.00

UNITS
RHC       PPM          1.0000     .0000     .0000
END                     .0000     .0000     .0000
```

Exhibit VII-2 (Continued)

```
STATIONS
        101     19183.     27862.      10.00
        102     17518.     34045.      10.00
        103     22588.     30467.      10.00
        104     22312.     25304.      10.00
        105     18706.     24453.      10.00
        106     13660.     25566.      10.00
        107     15179.     30610.      10.00
        108     23407.     39102.      10.00
        109     30802.     27886.      10.00
        110     22209.     20826.      10.00
        111     13812.     20479.      10.00
        112      8938.     28913.      10.00
        113     12738.     37820.      10.00
        114     19320.     45456.      10.00
        115     32111.     45799.      10.00
        116     37777.     38083.      10.00
        117     35560.     20818.      10.00
        118     18065.     11256.      10.00
        119      4759.     18547.      10.00
        120     -1921.     33909.      10.00
        121      7414.     50376.      10.00
        122     16631.     77223.      10.00
        123     52320.     34378.      10.00
        124     24275.    -15463.      10.00
        125    -27555.     30240.      10.00
 END                0.         0.        .00
```

Exhibit VII-2 (Continued)

```
TIME INTERVAL
     76195       500      76195       501
SUBREGION
A                  1          1        -1
END                0          0         0
METHOD
A         NO          POISSON        .0010    1.0000          3
MAXITER    1000.0000
ERRORTOL        .0010
OMEGA          1.4000
A         NO2         POISSON        .0010    1.0000          3
MAXITER    1000.0000
ERRORTOL        .0010
OMEGA          1.4000
A         O3          POISSON        .0010    1.0000          3
MAXITER    1000.0000
ERRORTOL        .0010
OMEGA          1.4000
A         RHC         POISSON        .0500    4.0000          3
MAXITER    1000.0000
ERRORTOL        .0500
OMEGA          1.4000
A         ETH          SPLIT/COMB    .0010    4.0000          1
RHC             .0217
A         OLE          SPLIT/COMB    .0010    4.0000          1
RHC             .0440
A         PAR          SPLIT/COMB    .0100    4.0000          1
RHC             .6665
A         CARB         SPLIT/COMB    .0010    4.0000          1
RHC             .0810
A         ARO          SPLIT/COMB    .0001    4.0000          1
RHC             .0248
A         BZA          SPLIT/COMB    .0000    4.0000          1
RHC             .0001
A         PAN           CONSTANT     .0000     .1000          0
A         CO            POISSON      .1000   20.0000          3
MAXITER    1000.0000
ERRORTOL        .1000
OMEGA          1.4000
                                     .0000     .0000          0
END
```

Exhibit VII-2 (Continued)

```
                                        METHODS TABLE

SUBREGION     VARIABLE      METHOD          MIN. VALUE     MAX. VALUE     PARAMETER      PAR. VALUE

A             NO            POISSON            .0010         1.0000
                                                                          MAXITER        1000.0000
                                                                          ERRORTOL           .0010
                                                                          OMEGA             1.4000
A             NO2           POISSON            .0010         1.0000
                                                                          MAXITER        1000.0000
                                                                          ERRORTOL           .0010
                                                                          OMEGA             1.4000
A             O3            POISSON            .0010         1.0000
                                                                          MAXITER        1000.0000
                                                                          ERRORTOL           .0010
                                                                          OMEGA             1.4000
A             ETH           SPLIT/COMB         .0010         4.0000
                                                                          RHC                .0217
A             OLE           SPLIT/COMB         .0010         4.0000
                                                                          RHC                .0440
A             PAR           SPLIT/COMB         .0100         4.0000
                                                                          RHC                .6665
A             CARB          SPLIT/COMB         .0010         4.0000
                                                                          RHC                .0810
A             ARO           SPLIT/COMB         .0001         4.0000
                                                                          RHC                .0248
A             BZA           SPLIT/COMB         .0000         4.0000
                                                                          RHC                .0001
A             PAN           CONSTANT           .0000          .1000
A             CO            POISSON            .1000        20.0000
                                                                          MAXITER        1000.0000
                                                                          ERRORTOL           .1000
                                                                          OMEGA             1.4000
A             RHC           POISSON            .0500         4.0000
                                                                          MAXITER        1000.0000
                                                                          ERRORTOL           .0500
                                                                          OMEGA             1.4000

VERTICAL METHOD
ALL       ALL         RELPROFRAT      .0000  100.0000         0
END                                   .0000     .0000         0
```

Exhibit VII-2 (Continued)

```
                                METHODS TABLE
SUBREGION    VARIABLE     METHOD      MIN. VALUE   MAX. VALUE   PARAMETER    PAR. VALUE

A            NO           RELPROFRAT     .0000      100.0000
A            NO2          RELPROFRAT     .0000      100.0000
A            O3           RELPROFRAT     .0000      100.0000
A            ETH          RELPROFRAT     .0000      100.0000
A            OLE          RELPROFRAT     .0000      100.0000
A            PAR          RELPROFRAT     .0000      100.0000
A            CARB         RELPROFRAT     .0000      100.0000
A            ARO          RELPROFRAT     .0000      100.0000
A            BZA          RELPROFRAT     .0000      100.0000
A            PAN          RELPROFRAT     .0000      100.0000
A            CO           RELPROFRAT     .0000      100.0000
A            RHC          RELPROFRAT     .0000      100.0000
CONSTANTS
A        PAN             .0000
END                      .0000
```

Exhibit VII-2 (Continued)

```
STATION READINGS                                      INITIAL COND  500
 101      03          .0240
 102      03       -9.0000
 103      03          .0270
 104      03       -9.0000
 105      03          .0020
 106      03          .0220
 107      03          .0300
 108      03          .0270
 109      03          .0380
 110      03          .0350
 111      03       -9.0000
 112      03          .0280
 113      03          .0340
 114      03          .0360
 115      03       -9.0000
 116      03          .0350
 117      03          .0360
 118      03       -9.0000
 119      03          .0290
 120      03          .0190
 121      03          .0020
 122      03          .0430
 123      03       -9.0000
 124      03          .0240
 125      03          .0030
 101      CO          .2540
 102      CO          .0500
 103      CO          .1740
 104      CO       -9.0000
 105      CO          .0500
 106      CO          .1850
 107      CO          .2260
 108      CO          .0550
 109      CO          .0500
 110      CO       -9.0000
 111      CO          .0590
 112      CO          .2670
 113      CO          .2090
 114      CO          .1090
 115      CO          .0500
 116      CO       -9.0000
 117      CO          .1480
 118      CO          .0500
 119      CO          .3200
 120      CO          .2390
 121      CO          .1080
 122      CO          .0500
 123      CO          .1750
 124      CO          .2560
 125      CO          .0770
```

Exhibit VII-2 (Continued)

101	RHC	-9.0000
102	RHC	.1310
103	RHC	.0860
104	RHC	.1780
105	RHC	-9.0000
106	RHC	.1960
107	RHC	.1460
108	RHC	.0600
109	RHC	-9.0000
110	RHC	-9.0000
111	RHC	.0820
112	RHC	.1170
113	RHC	.0500
114	RHC	-9.0000
115	RHC	-9.0000
116	RHC	-9.0000
117	RHC	-9.0000
118	RHC	-9.0000
119	RHC	.0500
120	RHC	.4740
121	RHC	-9.0000
122	RHC	-9.0000
123	RHC	-9.0000
124	RHC	-9.0000
125	RHC	-9.0000
101	NO	.0020
102	NO	.0020
103	NO	.0030
104	NO	.0020
105	NO	-9.0000
106	NO	.0020
107	NO	.0030
108	NO	.0050
109	NO	.0020
110	NO	.0020
111	NO	.0020
112	NO	.0020
113	NO	.0030
114	NO	.0020
115	NO	.0020
116	NO	.0020
117	NO	.0020
118	NO	.0020

Exhibit VII-2 (Continued)

```
 119      NO              .0020
 120      NO              .0030
 121      NO              .0020
 122      NO              .0020
 123      NO              .0020
 124      NO              .0020
 125      NO              .0020
 101      NO2             .0200
 102      NO2             .0040
 103      NO2             .0100
 104      NO2           -9.0000
 105      NO2           -9.0000
 106      NO2             .0020
 107      NO2             .0110
 108      NO2             .0100
 109      NO2             .0020
 110      NO2             .0050
 111      NO2             .0180
 112      NO2             .0160
 113      NO2             .0100
 114      NO2             .0080
 115      NO2             .0020
 116      NO2             .0020
 117      NO2             .0020
 118      NO2             .0030
 119      NO2             .0110
 120      NO2             .0220
 121      NO2             .0050
 122      NO2             .0020
 123      NO2             .0020
 124      NO2             .0030
 125      NO2             .0020
END                       .0000
VERTICAL PROFILE
A         ALL        35296.0000 5038.0000         4
        0.        .0000
      100.        .0000
      120.       1.0000
      500.       1.0000
END                       .0000     .0000         0
ENDTIME
```

Exhibit VII-2 (Continued)

```
FILE NAME -- AIRQUALITY      INITIAL POLLUTANT CONCENTRATIONS  ST LOUIS  500  76195                                              PAGE  1
AIR QUALITY VALUES (IN PARTS PER MILLION) SPECIES NO          VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  5.02
 GRID CELL          1          2          3          4          5          6          7          8          9         10         11         12
    22          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
    21          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
    20          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0021      .0021      .0021
    19          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0021      .0021      .0021      .0021
    18          .0020      .0020      .0020      .0020      .0021      .0021      .0020      .0021      .0021      .0021      .0021      .0021
    17          .0020      .0020      .0020      .0021      .0021      .0021      .0020      .0021      .0022      .0021      .0022      .0022
    16          .0020      .0020      .0021      .0021      .0022      .0022      .0022      .0023      .0023      .0020      .0025      .0024
    15          .0020      .0020      .0021      .0022      .0023      .0024      .0024      .0026      .0026      .0028      .0033      .0029
    14          .0020      .0020      .0022      .0023      .0025      .0025      .0026      .0030      .0028      .0032      .0050      .0034
    13          .0020      .0020      .0022      .0024      .0030      .0026      .0024      .0026      .0026      .0020      .0033      .0030
    12          .0020      .0020      .0021      .0023      .0024      .0023      .0020      .0025      .0030      .0025      .0030      .0026
    11          .0020      .0020      .0020      .0021      .0022      .0021      .0021      .0022      .0020      .0020      .0020      .0021
    10          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0021      .0020      .0020      .0020      .0020
     9          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     8          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     7          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     6          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     5          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     4          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     3          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     2          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
     1          .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020      .0020
```

Exhibit VII-2 (Continued)

```
FILE NAME -- AIRQUALITY      INITIAL POLLUTANT CONCENTRATIONS  ST LOUIS  500  76195                                         PAGE  2

AIR QUALITY VALUES (IN PARTS PER MILLION) SPECIES NO        VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  5.02

 GRID CELL        13         14         15         16         17

     22         .0020      .0020      .0020      .0020      .0020

     21         .0020      .0020      .0020      .0020      .0020

     20         .0021      .0021      .0020      .0020      .0020

     19         .0021      .0021      .0021      .0020      .0020

     18         .0021      .0021      .0021      .0020      .0020

     17         .0021      .0021      .0021      .0020      .0020

     16         .0020      .0021      .0021      .0020      .0020

     15         .0025      .0022      .0021      .0020      .0020

     14         .0027      .0023      .0020      .0020      .0020

     13         .0026      .0023      .0021      .0020      .0020

     12         .0023      .0022      .0021      .0020      .0020

     11         .0020      .0020      .0020      .0020      .0020

     10         .0020      .0020      .0020      .0020      .0020

      9         .0020      .0020      .0020      .0020      .0020

      8         .0020      .0020      .0020      .0020      .0020

      7         .0020      .0020      .0020      .0020      .0020

      6         .0020      .0020      .0020      .0020      .0020

      5         .0020      .0020      .0020      .0020      .0020

      4         .0020      .0020      .0020      .0020      .0020

      3         .0020      .0020      .0020      .0020      .0020

      2         .0020      .0020      .0020      .0020      .0020

      1         .0020      .0020      .0020      .0020      .0020
```

Exhibit VII-2 (Concluded)

B. BOUNDARY

The BOUNDARY file contains a time-invariant definition of the boundaries of the region to be modeled and time-varying matrices of pollutant concentrations in each external boundary cell. These boundary values are used by the Airshed Simulation Program to represent pollutant concentrations passing over the boundary into the modeling region. The program BNDARY is used to create the BOUNDARY file. BNDARY requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-3 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the BNDARY program.

1. Variables

The output variables for the BOUNDARY file are the species named in the CONTROL packet. Additional user-defined input variables (e.g., "reactive hydrocarbons") can be specified in the UNITS packet. The internal units for the concentrations of all species except AEROSOLS are parts per million (ppm); for AEROSOLS, the units are micrograms per cubic meter ($\mu g/m^3$). The standard names for reactive species recognized by the Airshed Simulation Program are listed in Section IX.A. If any of these species does not appear on the BOUNDARY file, the boundary concentrations will default to a value defined in the CHEMPARAM file. If any additional species appear on BOUNDARY, they will be ignored.

2. Methods

The methods that can be used to generate the BOUNDARY file are:

> CONSTANT
> BOUNDVALUE
> SPLIT/COMB
> USER.

The methods CONSTANT and BOUNDVALUE are equivalent. All these methods are discussed in detail in Section VI.A.6.

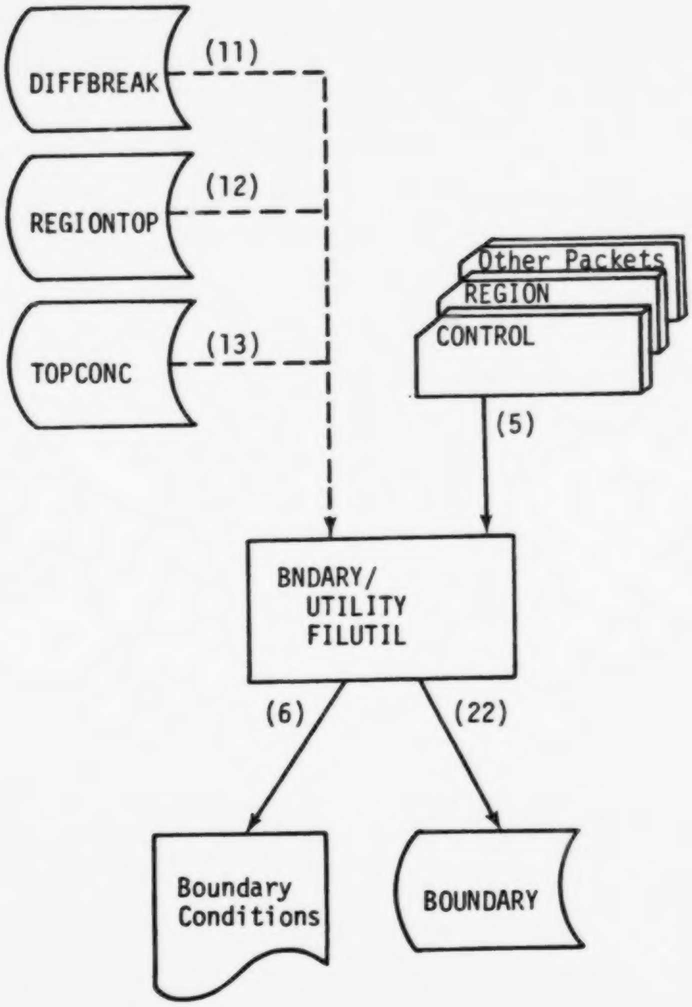

DIFFBREAK
(11)
REGIONTOP
(12)
TOPCONC
(13)
Other Packets
REGION
CONTROL
(5)
BNDARY/
UTILITY
FILUTIL
(6)
(22)
Boundary
Conditions
BOUNDARY

Figure VII-3. Information Flow Diagram for the BOUNDARY File

Since the BOUNDARY file varies in the vertical direction, a vertical method must also be specified for each output variable in each subregion. The vertical methods that can be used are:

- > CONSTANT
- > ABSPROFILE
- > RELPROFILE
- > ABSPROFRAT
- > RELPROFRAT
- > VERTUSER.

These vertical methods are discussed in detail in Section VI.A.7.

3. Time Variation

The time span of the BOUNDARY file must include the entire time span of the simulation runs for which it is to be used. Boundary concentrations are considered to be constant during each time interval.

4. Packets

Figure VII-4 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the BOUNDARY file:

- > CONTROL
  - The file name on Card 2 must be BOUNDARY.
  - The control variables to be specified on Cards 4 to 8 for BOUNDARY are shown in Table VII-2.
  - The number of species must be greater than zero.
  - If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.

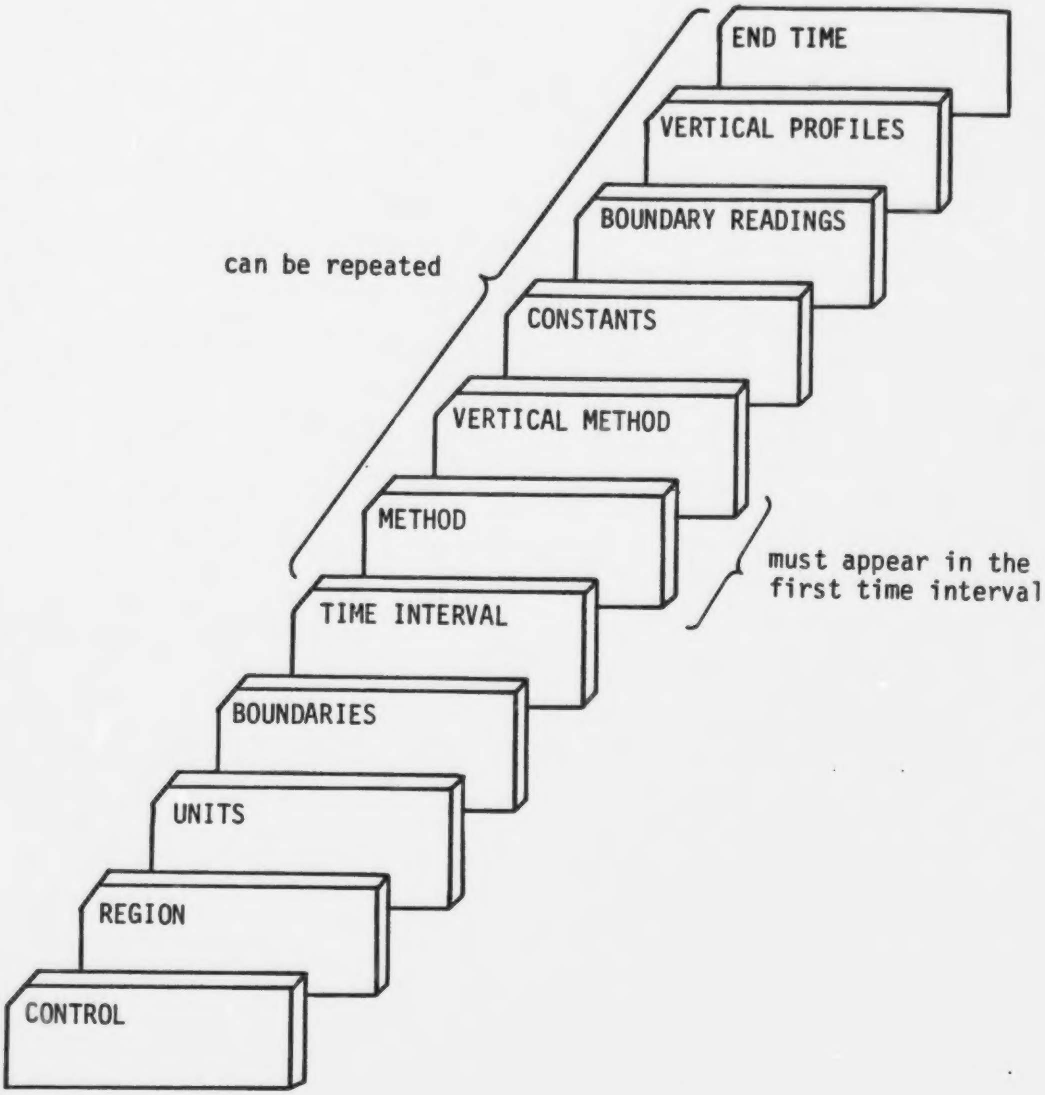

END TIME
VERTICAL PROFILES
BOUNDARY READINGS
can be repeated
CONSTANTS
VERTICAL METHOD
METHOD
must appear in the first time interval
TIME INTERVAL
BOUNDARIES
UNITS
REGION
CONTROL

Figure VII-4. Input Card Deck Structure for Preparing the BOUNDARY File

Table VII-2. CONTROL Packet Entries for the BOUNDARY File

Card Number	Entry
4	Number of species
	Number of user-defined variables
	Number of boundary line segments
	Spare
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output boundary values
	Spare
	Spare
	Spare
6	Print units table
	Print boundary line segment locations table
	Print regional grid
	Print methods table
	Print boundary values table
	Spare
7	Number of vertical parameters
	Number of heights in profile
	Print vertical methods table
	Print vertical profile tables
	Spare
	Spare
8	DIFFBREAK file number
	REGIONTOP file number
	TOPCONC file number
	Spare
	Spare
	Spare

- The number of boundary line segments must be at least three.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) must include maximum vertical parameter and profile entries as applicable.
- The file unit assignment card (No. 8) must provide entries for the DIFFBREAK, REGIONTOP, and TOPCONC files if, and only if, these files are required by the vertical methods selected.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is required; their number must be the same as the entry in the first control parameter on Card 4. If either the ABSPROFRAT or RELPROFRAT vertical method is selected for any variable, the output species names specified here must match the species names on the TOPCONC file.

> REGION. This packet must follow the CONTROL packet. The vertical parameters must be provided for the BOUNDARY file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:

- Any input variable will be input in other than internal units.
- Any user-defined variables are specified.
- COORD or HEIGHT unit conversions are to be used.

The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> BOUNDARIES. This packet is required; it names the line segments that define the boundaries of the region. The number of line segments specified must equal the number specified in the CONTROL packet.

> TIME INTERVAL. One or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> METHOD. A method must be provided for every variable--including user-defined variables--for every boundary line segment in the first time interval. In the METHOD packet, the boundary line segment name is entered in the "subregion" field. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> VERTICAL METHOD. A vertical method must be provided for every variable--including user-defined variables--for every boundary line segment in the first time interval. In the VERTICAL METHOD packet, the boundary line segment name is entered in the "subregion" field. Vertical methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each vertical parameter entry contributes to the overall vertical parameter count; the total must not exceed the maximum specified in the CONTROL packet.

> CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.

> BOUNDARY READINGS. If the method BOUNDVALUE is assigned to any variable in the METHOD packet, the first time interval must contain a BOUNDARY READINGS packet. More than one BOUNDARY READINGS packet can appear in any time interval.

> VERTICAL PROFILES. If any of the profile methods are assigned to any species in the VERTICAL METHOD packet, the first time interval must contain a VERTICAL PROFILES packet. There must be a vertical profile defined (or implied using ALL) for every variable for every boundary line segment for which a profile method was specified. In the VERTICAL PROFILES packet, the boundary line segment name is entered in the "subregion" field. The number of height-value pairs in any single profile must not exceed the maximum specified in the CONTROL packet. More than one VERTICAL PROFILES packet can appear in any time interval.

5. Additional Input Files

If any vertical method besides CONSTANT was selected, the DIFFBREAK and REGIONTOP files must be input to BNDARY. In addition, if the vertical method ABSPROFRAT or RELPROFRAT was selected, the TOPCONC file must also be input.

6. Examples

Exhibit VII-3 shows a sample input deck for BOUNDARY file generation. The output from a BNDARY run using that input deck is shown in Exhibit VII-4.

```
CONTROL
BOUNDARY
BOUNDARY DEFINITION AND CONCENTRATIONS
        11         1         4         1        10
        22         1         1
         1         1         1
         5         5                   0
        11        12        13
NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
     76195       500     76195      2400
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.       50.      200.
END
UNITS
RHC       PPM                1.
END
BOUNDARIES
TOP         -13000.    66000.    43000.    66000.
BOTTOM      -13000.   -10000.    43000.   -10000.
LEFT        -13000.   -10000.   -13000.    66000.
RIGHT        43000.   -10000.    43000.    66000.
END
```

Exhibit VII-3. Sample Input Deck for the BNDARY Program

```
TIME INTERVAL
     76195       500     76195       600
METHOD
ALL        NO          BOUNDVALUE     0.0          90.
ALL        NO2         BOUNDVALUE     0.0          90.
ALL        O3          BOUNDVALUE     0.0          90.
ALL        RHC         BOUNDVALUE     0.0          90.
ALL        PAN         BOUNDVALUE     0.0          90.
ALL        CO          BOUNDVALUE     0.0          90.
ALL        ETH         SPLIT/COMB     0.0          10.          1
RHC              .0217
ALL        OLE         SPLIT/COMB     0.0          10.          1
RHC              .0440
ALL        PAR         SPLIT/COMB     0.001        10.          1
RHC              .6665
ALL        CARB        SPLIT/COMB     0.0          10.          1
RHC              .0810
ALL        ARO         SPLIT/COMB     0.0          10.          1
RHC              .0248
ALL        BZA         SPLIT/COMB     0.0          10.          1
RHC              .0001
END
VERTICAL METHOD
ALL        ALL         RELPROFRAT     .0000       100.0
END
```

Exhibit VII-3 (Continued)

```
BOUNDARYREADINGS .
ALL       PAN      .00001
TOP       03            .023
RIGHT     03            .026
BOTTOM    03            .026
LEFT      03            .023
TOP       CO            .121
RIGHT     CO            .192
BOTTOM    CO            .192
LEFT      CO            .121
TOP       RHC           .079
RIGHT     RHC           .050
BOTTOM    RHC           .050
LEFT      RHC           .079
TOP       NO            .003
RIGHT     NO            .002
BOTTOM    NO            .002
LEFT      NO            .003
TOP       NO2           .007
RIGHT     NO2           .002
BOTTOM    NO2           .002
LEFT      NO2           .007
END
VERTICAL PROFILE
ALL       ALL          35296.     5038.      4
        0.       0.
      102.       0.
      122.       1.
     5000.       1.
END
ENDTIME
```

Exhibit VII-3 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE BOUNDARY

BOUNDARY DEFINITION AND CONCENTRATIONS


NUMBER OF USER-DEFINED VARIABLES =          1

NUMBER OF BOUNDARY LINES =          4

NUMBER OF METHOD PARAMETERS =         10

NUMBER OF VERTICAL METHOD PARAMETERS =          5

NUMBER OF VERTICAL PROFILE HEIGHTS =          5

PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER        22

INPUT DATA FOR DIFFUSION BREAK WILL BE OBTAINED FROM FILE NUMBER        11

INPUT DATA FOR REGION TOP WILL BE OBTAINED FROM FILE NUMBER        12

INPUT DATA FOR TOP CONCENTRATIONS WILL BE OBTAINED FROM FILE NUMBER        13

INPUT CARDS WILL BE PRINTED

OUTPUT GRID WILL BE PRINTED

UNIT TABLE WILL BE PRINTED

BOUNDARY LINE TABLE WILL BE PRINTED

BOUNDARY LINE MAP WILL BE PRINTED

INPUT VALUES METHOD TABLE WILL NOT BE PRINTED

BOUNDARY VALUES WILL NOT BE PRINTED

VERTICAL METHOD TABLE WILL NOT BE PRINTED

VERTICAL PROFILE VALUES WILL NOT BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       5.00

ENDING DATE OF FILE      76195 ENDING TIME OF FILE      24.00
```

Exhibit VII-4. Sample Output from BNDARY Program

```
A TOTAL OF        11 SPECIES NAMES WERE READ, THE SPECIES NAMES ARE --

NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
REGION
   725000.  4252000.        15
   -19000.    -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
```

Exhibit VII-4 (Continued)

```
                                          UNIT CONVERSION TABLE
VARIABLE NAME          UNIT NAME          MULTIPLICATIVE FACTOR  ADDITIVE FACTOR

     NO                                         -9.00000000        -9.00000000        -9.00000000
     NO2                                        -9.00000000        -9.00000000        -9.00000000
     O3                                         -9.00000000        -9.00000000        -9.00000000
     ETH                                        -9.00000000        -9.00000000        -9.00000000
     OLE                                        -9.00000000        -9.00000000        -9.00000000
     PAR                                        -9.00000000        -9.00000000        -9.00000000
     CARB                                       -9.00000000        -9.00000000        -9.00000000
     ARO                                        -9.00000000        -9.00000000        -9.00000000
     BZA                                        -9.00000000        -9.00000000        -9.00000000
     PAN                                        -9.00000000        -9.00000000        -9.00000000
     CO                                         -9.00000000        -9.00000000        -9.00000000
     RHC                  PPM                    1.00000000        -9.00000000        -9.00000000
     COORD                                      -9.00000000        -9.00000000        -9.00000000
     HEIGHT                                     -9.00000000        -9.00000000        -9.00000000
BOUNDARIES
TOP            -13000.    66000.    43000.    66000.
BOTTOM         -13000.   -10000.    43000.   -10000.
LEFT           -13000.   -10000.   -13000.    66000.
RIGHT           43000.   -10000.    43000.    66000.
END                 0.        0.        0.        0.
```

Exhibit VII-4 (Continued)

```
                                    BOUNDARY LINE LOCATION TABLE

B. LINE NAME      X-BEGINNING(GRID SQ)   X-ENDING (GRID SQ)   Y-BEGINNING (GRID SQ)   Y-ENDING(GRID SQ)

   TOP                     1.50                15.50                 20.50                20.50

   BOTTOM                  1.50                15.50                  1.50                 1.50

   LEFT                    1.50                 1.50                  1.50                20.50

   RIGHT                  15.50                15.50                  1.50                20.50

****** NOTE ******  BOUNDARY LINES LEFT       AND BOTTOM     INTERSECT IN CELL (        2,         2).

THIS CELL WILL TAKE ITS VALUE FROM THE LATTER LINE

****** NOTE ******  BOUNDARY LINES RIGHT      AND BOTTOM     INTERSECT IN CELL (       16,         2).

THIS CELL WILL TAKE ITS VALUE FROM THE LATTER LINE

****** NOTE ******  BOUNDARY LINES LEFT       AND TOP        INTERSECT IN CELL (        2,        21).

THIS CELL WILL TAKE ITS VALUE FROM THE LATTER LINE

****** NOTE ******  BOUNDARY LINES RIGHT      AND TOP        INTERSECT IN CELL (       16,        21).

THIS CELL WILL TAKE ITS VALUE FROM THE LATTER LINE
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS                                               PAGE  1

MAP OF BOUNDARY LINE NUMBERS ON THE REGIONAL GRID          VERT.  LEVEL 0 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195 24.00

 GRID CELL    1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16   17

    22        0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0

    21        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0

    20        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    19        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    18        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    17        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    16        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    15        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    14        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    13        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    12        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    11        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

    10        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     9        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     8        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     7        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     6        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     5        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     4        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     3        0    3    0    0    0    0    0    0    0    0    0    0    0    0    0    4    0

     2        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0

     1        0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
```

Exhibit VII-4 (Continued)

```
BOUNDARY LINE IDENTIFICATION

   NUMBER        NAME


         1     TOP

         2     BOTTOM

         3     LEFT

         4     RIGHT

TIME INTERVAL
      76195        500      76195        600
     ** READING DIFFBREAK FILE : DATE= 76195   TIME=     5.00 **
     ** READING REGNTOP   FILE : DATE= 76195   TIME=     5.00 **
     ** READING TOPCONC   FILE : DATE= 76195   TIME=     5.00 **
METHOD
ALL       NO          BOUNDVALUE      .0000   90.0000           0
ALL       NO2         BOUNDVALUE      .0000   90.0000           0
ALL       O3          BOUNDVALUE      .0000   90.0000           0
ALL       RHC         BOUNDVALUE      .0000   90.0000           0
ALL       PAN         BOUNDVALUE      .0000   90.0000           0
ALL       CO          BOUNDVALUE      .0000   90.0000           0
ALL       ETH         SPLIT/COMB      .0000   10.0000           1
RHC               .0217
ALL       OLE         SPLIT/COMB      .0000   10.0000           1
RHC               .0440
ALL       PAR         SPLIT/COMB      .0010   10.0000           1
RHC               .6665
ALL       CARB        SPLIT/COMB      .0000   10.0000           1
RHC               .0810
ALL       ARO         SPLIT/COMB      .0000   10.0000           1
RHC               .0248
ALL       BZA         SPLIT/COMB      .0000   10.0000           1
RHC               .0001
END                                   .0000     .0000           0
VERTICAL METHOD
ALL       ALL         RELPROFRAT      .0000  100.0000           0
END                                   .0000     .0000           0
```

Exhibit VII-4 (Continued)

```
BOUNDARYREADINGS
ALL       PAN           .0000
TOP       O3            .0230
RIGHT     O3            .0260
BOTTOM    O3            .0260
LEFT      O3            .0230
TOP       CO            .1210
RIGHT     CO            .1920
BOTTOM    CO            .1920
LEFT      CO            .1210
TOP       RHC           .0790
RIGHT     RHC           .0500
BOTTOM    RHC           .0500
LEFT      RHC           .0790
TOP       NO            .0030
RIGHT     NO            .0020
BOTTOM    NO            .0020
LEFT      NO            .0030
TOP       NO2           .0070
RIGHT     NO2           .0020
BOTTOM    NO2           .0020
LEFT      NO2           .0070
END                     .0000
VERTICAL PROFILE
ALL       ALL      35296.0000 5038.0000         4
        0.      .0000
      102.      .0000
      122.     1.0000
     5000.     1.0000
END                     .0000     .0000         0
ENDTIME
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS
                                                                                                         PAGE  1
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO        VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL          1         2         3         4         5         6         7         8         9        10        11        12
      4       -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      3       -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      2       -9.0000     .0020     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030
      1       -9.0000     .0020     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS                                                  PAGE  2
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO        VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL       13        14        15        16        17        18        19        20        21        22
     4         .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010   -9.0000
     3         .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010   -9.0000
     2         .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030   -9.0000
     1         .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030   -9.0000
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY      BOUNDARY DEFINITION AND CONCENTRATIONS                                                      PAGE  1
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO        VERT.  LEVEL 2 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL         1         2         3         4         5         6         7         8         9        10        11        12
      4      -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      3      -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      2      -9.0000     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020
      1      -9.0000     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS                                                    PAGE  2

BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO         VERT.  LEVEL 2 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00

 GRID CELL        13        14        15        16        17        18        19        20        21        22

      4         .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010   -9.0000

      3         .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010   -9.0000

      2         .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0030   -9.0000

      1         .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0030   -9.0000
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY      BOUNDARY DEFINITION AND CONCENTRATIONS
                                                                                                              PAGE  1
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO        VERT.  LEVEL 3 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL         1         2         3         4         5         6         7         8         9        10        11        12
      4     -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      3     -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      2     -9.0000     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020
      1     -9.0000     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020     .0020
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS                                        PAGE  2
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO        VERT.  LEVEL 3 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL       13        14        15        16        17
      4        .0010     .0010     .0010     .0010   -9.0000
      3        .0010     .0010     .0010     .0010   -9.0000
      2        .0020     .0020     .0020     .0020   -9.0000
      1        .0020     .0020     .0020     .0020   -9.0000
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS                                                      PAGE  1
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO        VERT.  LEVEL 4 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        1         2         3         4         5         6         7         8         9        10        11        12
      4      -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      3      -9.0000     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010     .0010
      2      -9.0000     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030
      1      -9.0000     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030     .0030
```

Exhibit VII-4 (Continued)

```
FILE NAME -- BOUNDARY       BOUNDARY DEFINITION AND CONCENTRATIONS                                                    PAGE  2
BOUNDARY CONCENTRATIONS (PARTS PER MILLION) FOR   NO          VERT.  LEVEL 4 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        13        14        15        16        17
      4         .0010     .0010     .0010     .0010   -9.0000
      3         .0010     .0010     .0010     .0010   -9.0000
      2         .0030     .0030     .0030     .0030   -9.0000
      1         .0030     .0030     .0030     .0030   -9.0000
```

Exhibit VII-4 (Concluded)

C. DIFFBREAK

The DIFFBREAK file contains time-varying two-dimensional matrices of diffusion break heights. The diffusion break is used to define the distribution of cells in the vertical direction and to delimit layers of the atmosphere with different diffusion characteristics. The diffusion break is usually set to the mixing height or the height of the inversion base. The program DFSNBK is used to create the DIFFBREAK file. DFSNBK requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-5 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the DFSNBK program.

1. Variables

The output variable for the DIFFBREAK file is also named DIFFBREAK. This is an "implicit output variable" and need not be referred to anywhere in the CONTROL packet. The internal units for DIFFBREAK are meters (m). If the input values for this variable are to be in any other units, DIFFBREAK must be specified in the UNITS packet.

2. Methods

The methods that can be used to generate the DIFFBREAK file are:

> CONSTANT
> GRID VALUE
> STATINTERP
> POISSON
> E-WINTERP
> N-SINTERP
> USER.

These methods are discussed in detail in Section VI.A.6.

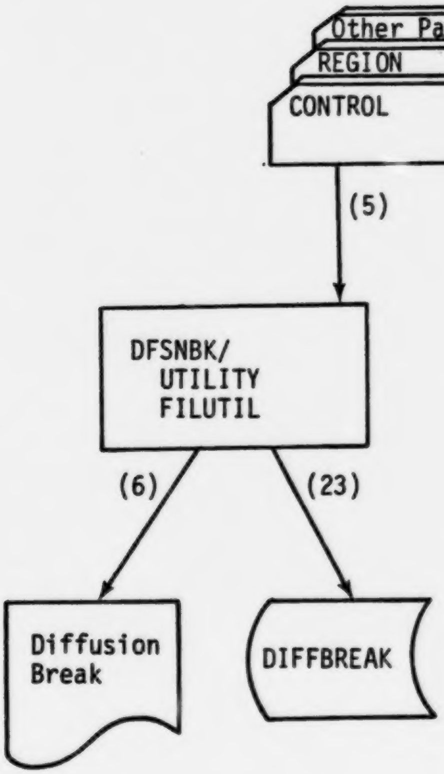

Other Packets
REGION
CONTROL
(5)
DFSNBK/
UTILITY
FILUTIL
(6)
(23)
Diffusion
Break
DIFFBREAK

Figure VII-5. Information Flow Diagram for the DIFFBREAK File

3. Time Variation

The diffusion break values on the DIFFBREAK file are considered to apply at the beginning of the time interval. Because the Airshed Simulation Program calculates diffusion break values continuously over time by linear interpolation, it also requires values at the end of the time interval. These are read by the program as the values at the beginning of the next time interval. Thus, the last time interval on the file must begin at or after the ending simulation time. For example, if a simulation is to be made from 0500-1700, and diffusion break values are input hourly, the values used between 500 and 600 are calculated by interpolating between values input for the 0500-0600 time interval and those input for the 0600-0700 time interval. Similarly, to calculate values between 1600 and 1700, the simulation program requires values for the interval 1600-1700 as well as another set for an interval beginning at 1700.

4. Packets

Figure VII-6 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the DIFFBREAK file:

> CONTROL

- The file name on Card 2 must be DIFFBREAK.
- The control variables to be specified on Cards 4 to 8 for DIFFBREAK are shown in Table VII-3.
- The number of species should be zero.
- If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.

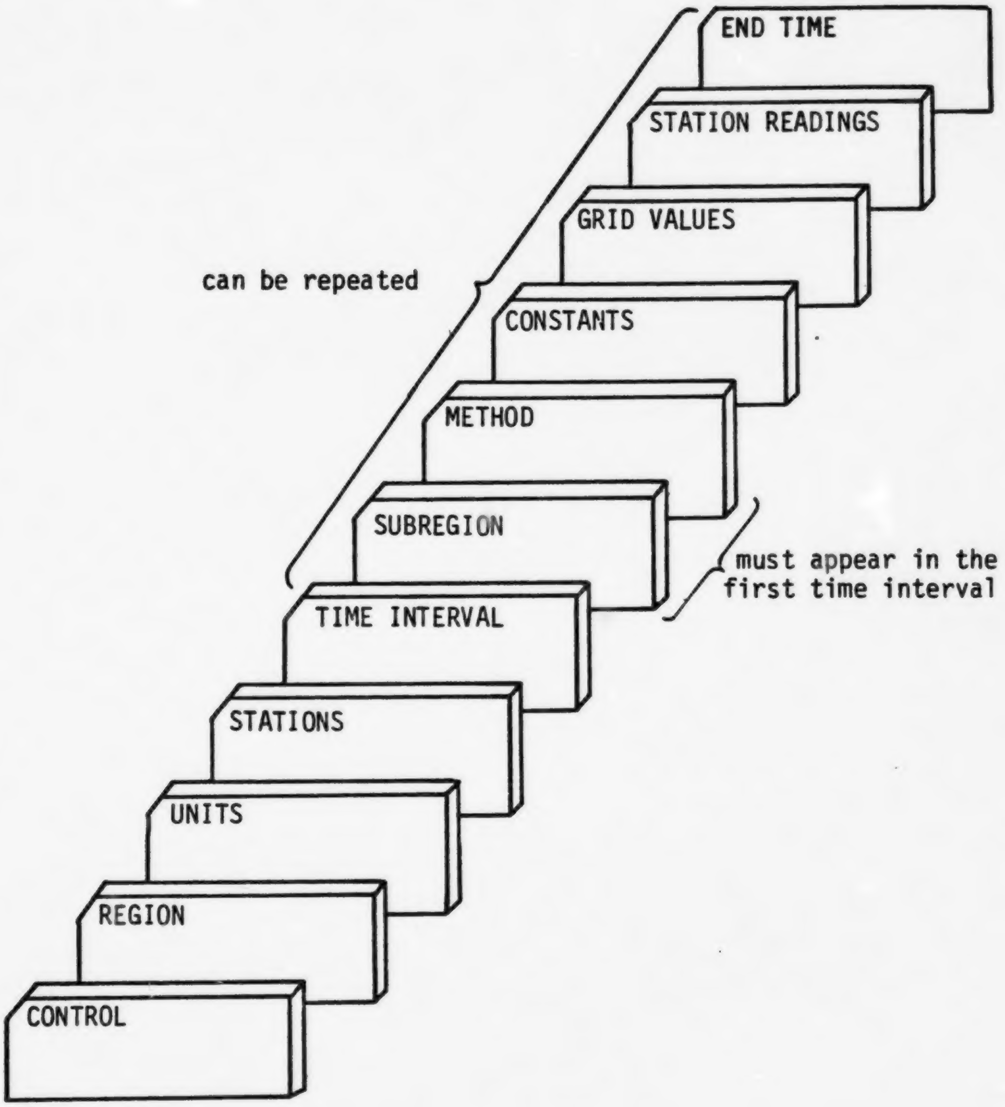

END TIME
STATION READINGS
GRID VALUES
can be repeated
CONSTANTS
METHOD
SUBREGION
must appear in the first time interval
TIME INTERVAL
STATIONS
UNITS
REGION
CONTROL

Figure VII-6. Input Card Deck Structure for Preparing the DIFFBREAK FILE

Table VII-3. CONTROL Packet Entries for the DIFFBREAK File

Number	Entry
4	Number of species (=0)
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
8	Spare
	Spare
	Spare
	Spare
	Spare
	Spare

- If data from measuring stations are to be used (methods STATINTERP or POISSON), the maximum number of such stations must be given.
- The number of subregions must be at least one.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) should be left blank.
- The file unit assignment card (No. 8) should be left blank.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is not required; if they are present, their number must be the same as the entry in the first control parameter on Card 4, but they will be ignored by the program.

> REGION. This packet must follow the CONTROL packet. The vertical parameters will be ignored for the DIFFBREAK file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:

- Any input variable will be input in other than internal units.
- Any user-defined variables are specified.
- COORD or HEIGHT unit conversions are to be used.

The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> STATIONS. This packet is required if either of the methods STATINTERP or POISSON is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.

> TIME INTERVAL. Two or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. The last time interval must begin at or

after the ending time of any simulation run. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> SUBREGION. The first time interval must contain a SUBREGION packet; the inclusion of this packet in other time intervals is optional. The number of subregions must not exceed the maximum specified in the CONTROL packet.

> METHOD. A method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.

> GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, the first time interval must contain a GRID VALUES packet. More than one GRID VALUES packet can appear in any time interval.

> STATION READINGS. If either the POISSON or STATINTERP method is assigned to any variable in the METHOD packet, the first time interval must contain a STATION READINGS packet. More than one STATION READINGS packet can appear in any time interval.

5. Additional Input Files

No additional input files are required.

6. Examples

Exhibit VII-5 shows a sample input deck for DIFFBREAK file generation. The output from a DFSNBK run using that input deck is shown in Exhibit VII-6.

```
CONTROL
DIFFBREAK
   HEIGHT OF THE MIXED LAYER
                            12         1        10
        23         1         1



     76195       500     76196        10
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.        50.      200.
END
STATIONS
 141          17949.    27053.
 141A         14000.    23000.
 141B         14000.    27000.
 141C         14000.    31000.
 141D         18000.    31000.
 141E         18000.    23000.
 141F         22000.    23000.
 141G         22000.    27000.
 141H         22000.    31000.
 142          -9294.    14115.
 143          35296.     5038.
 144          30861.    56067.
END
TIME INTERVAL
     76195       500     76195       600
SUBREGION
A                  1         1        -1
END
```

Exhibit VII-5. Sample Input Deck for the DFNSBK Program

```
METHOD
A          DIFFBREAK POISSON        0.      2000.        3
 RMAXIT       200.
 TLRNCE        0.5
 ROMEGA          1.4
END
STATION READINGS
 141       DIFFBREAK      402.
 141A      DIFFBREAK      402.
 141B      DIFFBREAK      402.
 141C      DIFFBREAK      402.
 141D      DIFFBREAK      402.
 141E      DIFFBREAK      402.
 141F      DIFFBREAK      402.
 141G      DIFFBREAK      402.
 141H      DIFFBREAK      402.
 142       DIFFBREAK     102.
 143       DIFFBREAK     102.
 144       DIFFBREAK     102.
 END
 ENDTIME
 TIME INTERVAL
      76195       600     76195       700
 STATION READINGS
  141       DIFFBREAK      418.
  141A      DIFFBREAK      418.
  141B      DIFFBREAK      418.
  141C      DIFFBREAK      418.
  141D      DIFFBREAK      418.
  141E      DIFFBREAK      418.
  141F      DIFFBREAK      418.
  141G      DIFFBREAK      418.
  141H      DIFFBREAK      418.
  142       DIFFBREAK     167.
  143       DIFFBREAK     167.
  144       DIFFBREAK     167.
 END
 ENDTIME
```

Exhibit VII-5 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE DIFFBREAK

   HEIGHT OF THE MIXED LAYER

NUMBER OF STATIONS =         12

NUMBER OF SUBREGIONS =          1

NUMBER OF METHOD PARAMETERS =         10

PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER         23

INPUT CARDS WILL BE PRINTED

OUTPUT GRID WILL BE PRINTED

UNIT TABLE WILL NOT BE PRINTED

STATION LOCATIONS WILL NOT BE PRINTED

SUBREGION GRID WILL NOT BE PRINTED

METHOD TABLE WILL NOT BE PRINTED

STATION VALUES WILL NOT BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       5.00

ENDING DATE OF FILE      76196 ENDING TIME OF FILE        .17

REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
```

Exhibit VII-6.   Sample Output from the DFNSBK Program

```
FILE NAME -- DIFFBREAK          HEIGHT OF THE MIXED LAYER                                                               PAGE  1
DIFFUSION BREAK VALUES (IN METERS ABOVE GROUND LEVEL)        VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL         1          2          3          4          5          6          7          8          9         10         11         12
      22    102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000
      21    102.0000   104.0061   105.9784   107.8764   109.6442   111.2035   112.4517   113.2621   113.4869   112.9678   111.5785   109.4017
      20    102.0000   106.0492   110.0391   113.8977   117.5229   120.7653   123.4199   125.2271   125.8663   124.9496   122.0040   116.6038
      19    102.0000   108.1576   114.2490   120.1900   125.8482   131.0156   135.3871   138.5582   140.0230   139.1342   134.8865   124.9782
      18    102.0000   110.3394   118.6380   126.8301   134.7796   142.2370   148.8003   153.8979   156.8324   156.8625   153.3217   145.7940
      17    102.0000   112.5715   123.1758   133.8129   144.3856   154.6312   164.0430   171.8205   176.9206   178.3270   175.4780   168.5566
      16    102.0000   114.7858   127.7453   141.0099   154.5890   168.2632   181.4332   192.9575   201.1329   204.1504   201.2368   192.7235
      15    102.0000   116.8553   132.1119   148.1159   165.0816   182.9509   201.1351   218.0985   230.9451   235.9049   231.8983   219.3304
      14    102.0000   118.5852   135.8983   154.5894   175.1980   198.0348   222.8621   248.0858   269.0660   276.4828   270.2190   249.5590
      13    102.0000   119.7123   138.5788   159.6205   183.7796   211.9917   245.0963   283.0558   321.0929   330.4662   321.8958   283.8507
      12    102.0000   119.9191   139.5127   162.1920   189.1754   222.0373   263.4087   318.6224   402.0000   402.0000   402.0000   318.1304
      11    102.0000   118.8524   137.9964   161.3214   189.7096   224.6137   268.7601   326.5473   402.0000   402.0000   402.0000   324.6042
      10    102.0000   116.1240   133.1719   156.4365   184.8351   218.9656   261.2449   317.1956   402.0000   402.0000   402.0000   313.3499
       9    102.0000   111.3740   123.2244   147.5830   175.3284   206.0785   240.6791   279.2575   317.1860   325.2433   314.3020   272.3603
       8    102.0000   105.3165   102.0000   136.5030   163.7951   190.0691   216.5829   242.1357   262.1583   267.2108   257.2377   231.7732
       7    102.0000   107.2511   114.7118   133.6508   154.0439   174.3307   193.7312   210.6377   222.0515   224.0679   215.5090   196.6989
       6    102.0000   108.3177   117.0373   130.1234   144.9114   159.7828   173.5247   184.6783   191.3240   191.4567   183.9997   168.4714
       5    102.0000   108.1039   115.7802   125.3862   135.9776   146.5089   155.9673   163.2427   167.1079   166.4374   160.5847   149.4631
       4    102.0000   107.0870   113.0524   119.9097   127.2197   134.3517   140.6021   145.2149   147.4289   146.6159   142.4751   135.1894
       3    102.0000   105.6063   109.6386   114.0663   118.6635   123.0710   126.8604   129.5737   130.7749   130.1351   127.5416   123.2044
       2    102.0000   103.8637   105.8902   108.0631   110.2833   112.3872   114.1739   115.4294   115.9563   115.6151   114.3737   112.3549
       1    102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000   102.0000
```

Exhibit VII-6 (Continued)

```
                                                                                                          PAGE  2
FILE NAME -- DIFFBREAK          HEIGHT OF THE MIXED LAYER
DIFFUSION BREAK VALUES (IN METERS ABOVE GROUND LEVEL)       VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        13        14        15        16        17
     22     102.0000  102.0000  102.0000  102.0000  102.0000
     21     107.2683  107.4373  107.3662  105.8242  102.0000
     20     109.6837  111.9638  112.2625  109.0659  102.0000
     19     102.0000  116.8009  118.0606  112.6005  102.0000
     18     135.3789  132.9462  127.3580  117.1122  102.0000
     17     158.9566  149.4731  137.5922  121.9777  102.0000
     16     180.1957  165.2262  147.5758  126.6674  102.0000
     15     201.3668  180.3163  156.8746  130.8992  102.0000
     14     223.0223  194.5563  165.1207  134.4611  102.0000
     13     244.1440  206.8965  171.6151  137.0459  102.0000
     12     260.6950  214.9730  175.1758  138.1938  102.0000
     11     263.9149  215.4856  174.4594  137.4240  102.0000
     10     253.7866  207.5854  168.9463  134.5254  102.0000
      9     229.6791  191.6240  158.8958  129.6244  102.0000
      8     200.6825  170.1863  145.3731  123.1938  102.0000
      7     171.0517  143.1141  129.3504  115.9792  102.0000
      6     143.7772  102.0000  113.1119  109.5702  102.0000
      5     133.6663  115.8389  111.6856  107.3430  102.0000
      4     125.6634  116.0918  110.5570  106.2150  102.0000
      3     117.7668  112.3746  108.3042  105.0166  102.0000
      2     109.8678  107.3805  105.3094  103.5776  102.0000
      1     102.0000  102.0000  102.0000  102.0000  102.0000
```

Exhibit VII-6 (Concluded)

D. EMISSIONS

The EMISSIONS file contains time-varying matrices of ground-level emission fluxes. At present, there is no general-purpose program for creating the EMISSIONS file because its generation is so highly dependent on the form of the emissions data available: traffic, stationary sources, area sources, airports, and so on. There is a program structure, similar to that of the other data preparation programs, that includes the reading of control packets, unit conversions, and writing the proper output records. This program can be tailored to particular input requirements as necessary. The skeleton program is named EMISSN. EMISSN requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-7 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the card input to the EMISSN program.

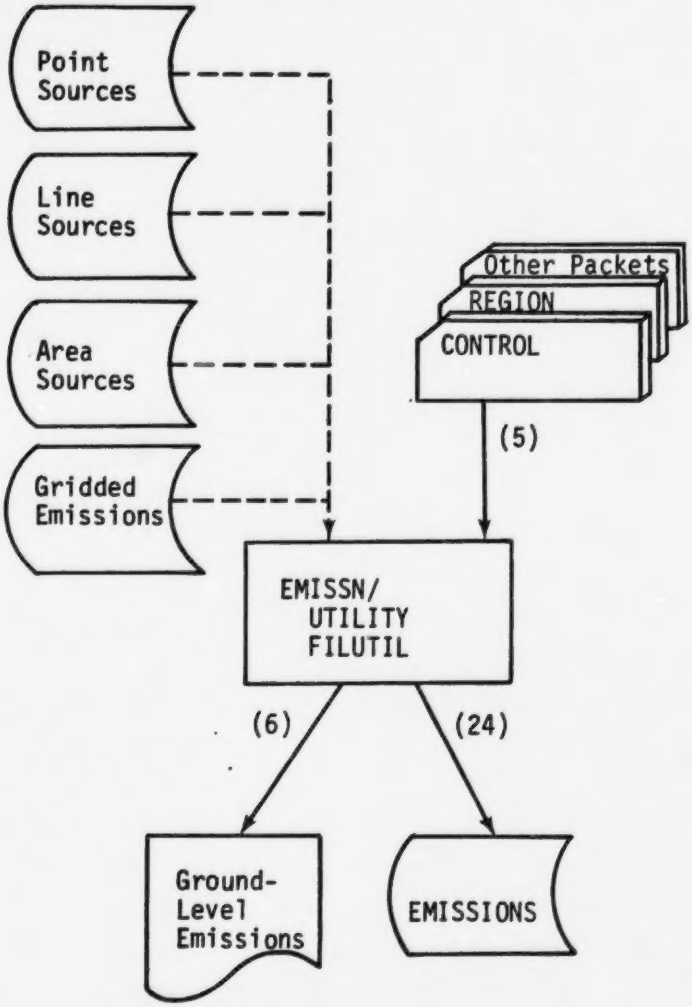
1. Variables

The output variables for the EMISSIONS file are the species named in the CONTROL packet. Additional user-defined input variables (e.g. "reactive hydrocarbons") can be specified in the UNITS packet. The internal units for ground-level emissions of all species except AEROSOLS are gram-moles per hour (g-mol/hr); for AEROSOLS, the units are grams per hour (g/hr). The standard names for reactive species recognized by the Airshed Simulation Program are listed in Section IX.A. If any of these species does not appear on the EMISSIONS file, the emissions values default to zero. If any additional species appear on EMISSIONS, they will be ignored.

2. Methods

The methods that can be used to generate the EMISSIONS file are:

> CONSTANT
> GRID VALUE
> SPLIT/COMB
> USER.



Point Sources
Line Sources
Area Sources
Gridded Emissions
Other Packets
REGION
CONTROL
(5)
EMISSN/ UTILITY FILUTIL
(6)
(24)
Ground-Level Emissions
EMISSIONS

Figure VII-7. Information Flow Diagram for the EMISSIONS File

The actual methods for generating output values from specific input data files must be written for each new application.

3. Time Variation

The time span of the EMISSIONS file must include the entire time span of the simulation runs for which it is to be used. Ground-level emissions are considered to be constant during each time interval.

4. Packets

The packets to be used for EMISSN will depend on the particular version that is developed for a given set of input data files. Information on control parameters, units, time intervals, computation methods, and data entry will have to be provided when the program has been implemented. Figure VII-8 shows a possible input structure in terms of the packets to be used.

5. Additional Input Files

Point source, line source, area source, or gridded area emissions might be input to EMISSN.

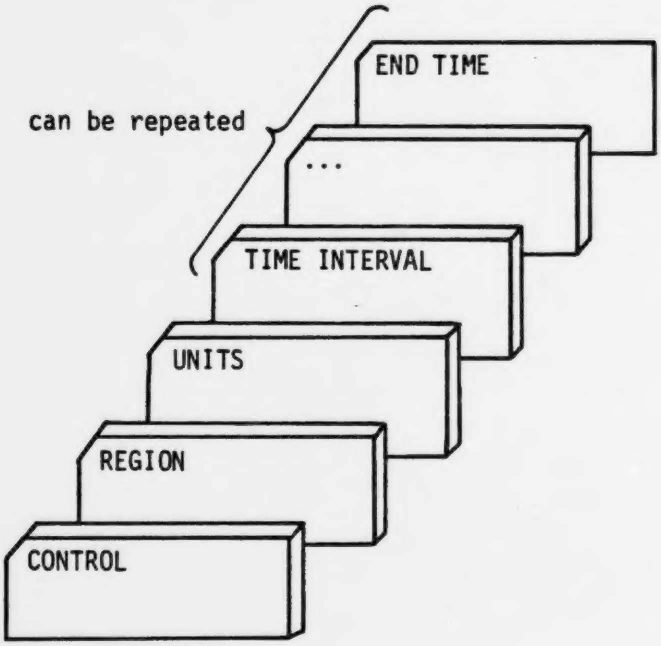

can be repeated
END TIME
...
TIME INTERVAL
UNITS
REGION
CONTROL

Figure VII-8. A Possible Input Card Deck Structure for Preparing the EMISSIONS File

E. METSCALARS

The METSCALARS file contains a set of time-varying scalars to be used in meteorological calculations. It has no spatial dependence. The program METSCL is used to create the METSCALARS file. METSCL requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-9 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the METSCL program.

1. Variables

There are six output variables for the METSCALARS file. Their names and internal units are:

- TGRADBELOW--temperature gradient below the diffusion break (°K/m).
- TGRADABOVE--temperature gradient above the diffusion break (°K/m).
- EXPCLASS--exposure class, an integer scale (+3 to -2) of the near ground-level atmospheric stability due to surface heating or cooling. It can be estimated from insolation as follows:

$$\text{exposure class} = \left\{ \begin{array}{l} \left.\begin{array}{ll} 3, & \text{strong} \\ 2, & \text{moderate} \\ 1, & \text{slight} \end{array}\right\} \quad \text{daytime insolation}, \\ \begin{array}{ll} 0, & \text{heavy overcast} \end{array} \quad \text{day or night}, \\ \left.\begin{array}{ll} -1, & \geq\frac{4}{8}\ \text{cloud cover} \\ -2, & \leq\frac{3}{8}\ \text{cloud cover} \end{array}\right\} \quad \text{nighttime cloudiness}. \end{array}\right.$$

- RADFACTOR--the NO_2 photolysis rate constant, k_1 (min^{-1}).
- CONCWATER--average concentration of water (ppm).
- ATMOSPRESS--atmospheric pressure (atm).

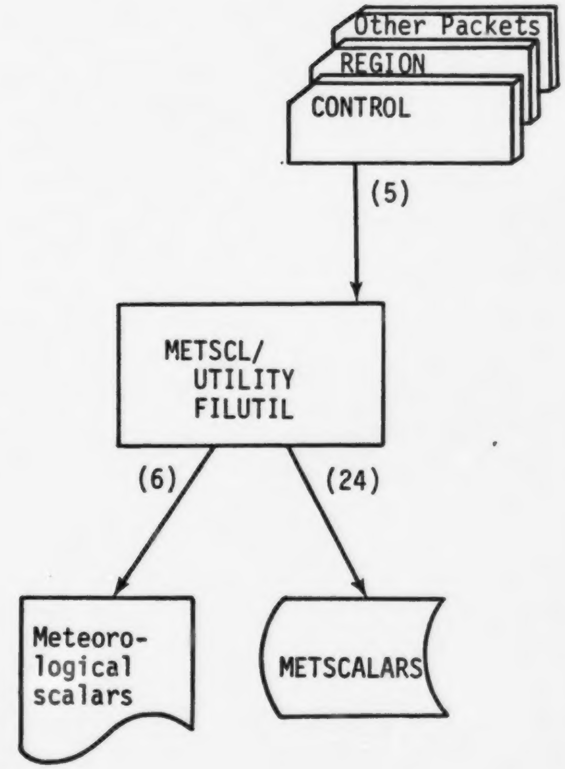

Other Packets
REGION
CONTROL
(5)
METSCL/
UTILITY
FILUTIL
(6)
(24)
Meteoro-
logical
scalars
METSCALARS

Figure VII-9. Information Flow Diagram for the METSCALARS File

2. Methods

Since the METSCALARS variables do not vary spatially, there is no need to define a method for determining spatial distribution. It is assumed that the variables will be explicitly entered in SCALARS packets and that only simple unit conversions, which are defined in the UNITS packet, need be performed.

3. Time Variation

Five of the METSCALARS variables, TGRADBELOW, TGRADABOVE, EXPCLASS, CONCWATER, and ATMOSPRESS, are considered to be constant during each time interval. The sixth variable, RADFACTOR, however, is considered to apply at the end of the time interval. Because the Airshed Simulation Program calculates radiation factor values continuously over time by linear interpolation, it also requires values at the beginning of the time interval. These are saved by the program as the values read for the end of the previous time interval. Thus the first time interval on the file must end at or before the beginning simulation time. For example, if a simulation is to be made from 0500-1700, and radiation factor values are input hourly, the values used between 500 and 600 are calculated by interpolating between values input for the 0400-0500 time interval and those input for the 0500-0600 time interval.

4. Packets

Figure VII-10 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Sections VI.B. Following are special input packet considerations for the file:

> CONTROL
  - The file name on Card 2 must be METSCALARS.
  - The control variables to be specified on Cards 4 to 8 for METSCALARS are shown in Table VII-4.

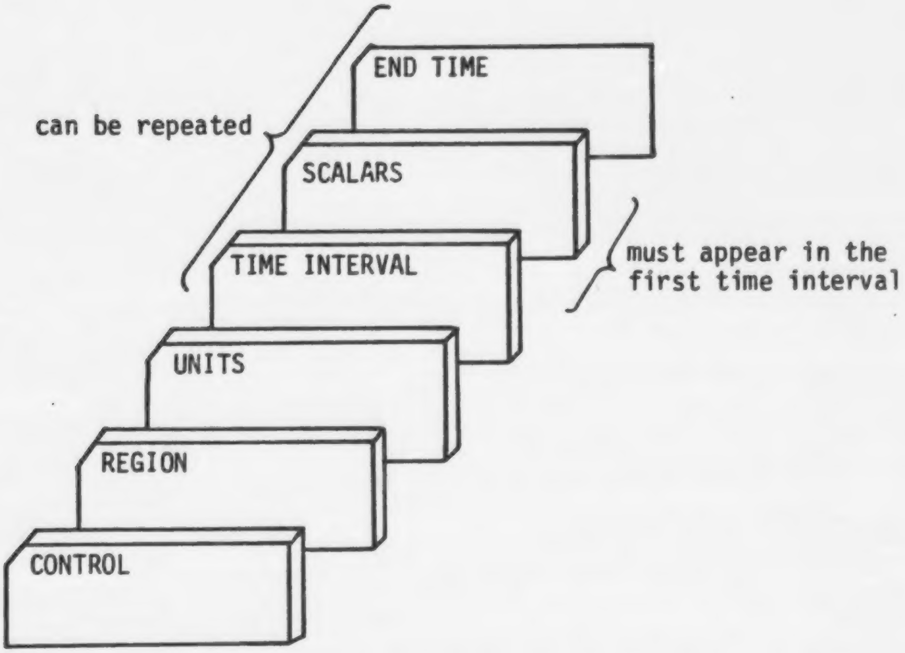

END TIME
SCALARS
TIME INTERVAL
UNITS
REGION
CONTROL
can be repeated
must appear in the first time interval

Figure VII-10. Input Card Deck Structure for Preparing the METSCALARS File

Table VII-4. CONTROL Packet Entries for the METSCALARS File

Card Number	Entry
4	Number of species (=0)
	Spare
	Spare
	Spare
	Spare
	Spare
5	Output file number
	Print input cards
	Print output values
	Spare
	Spare
	Spare
6	Print units table
	Spare
	Spare
	Spare
	Spare
	Spare
7	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
8	Spare
	Spare
	Spare
	Spare
	Spare
	Spare

- The number of species should be zero.
- The vertical controls card (No. 7) should be left blank.
- The file unit assignment card (No. 8) should be left blank.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is not required; if they are present, their number must be the same as the entry in the first control parameter on Card 4, but they will be ignored by the program.

> REGION. This packet must follow the CONTROL packet. The vertical parameters will be ignored for the METSCALARS file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if any input variable will be input in other than internal units. The units of RADFACTOR must be min^{-1} and cannot be changed.

> TIME INTERVAL. Two or more TIME INTERVAL packets must be present. The first time interval must end at or before the beginning time of any simulation run. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains a SCALARS packet and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> SCALARS. The first time interval must contain a SCALARS packet. Following the first time interval, the SCALARS packet can be omitted if no values are to be changed.

5. Additional Input Files

No additional input files are required.

6. Examples

Exhibit VII-7 shows a sample input deck for METSCALARS file generation. The output from a METSCL run using that input deck is shown in Exhibit VII-8.

```
CONTROL
MET SCALARS
    VALUES FOR METEOROLOGICAL SCALARS
         0         0         0         1         3
        24         1         1
         1


     76195       400     76195      2400
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.       50.      200.
END
TIMEINTERVAL
     76195       400     76195       500
SCALARS
TGRADBELOW    -0.01
TGRADABOVE    0.0039
EXPCLASS     -1.
ATMOSPRESS      0.99
RADFACTOR      .008
CONCWATER    12687.
END
ENDTIME
TIME INTERVAL
     76195       500     76195       600
SCALARS
RADFACTOR      .084
EXPCLASS       0.0
END
ENDTIME
TIME INTERVAL
     76195       600     76195       700
SCALARS
EXPCLASS       1.
CONCWATER    12687.
RADFACTOR      .180
END
ENDTIME
```

Exhibit VII-7. Sample Input Deck for the METSCL Program

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE METSCALARS

    VALUES FOR METEOROLOGICAL SCALARS

PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER        24

INPUT CARDS WILL BE PRINTED

OUTPUT GRID WILL BE PRINTED

UNIT TABLE WILL BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       4.00

ENDING DATE OF FILE      76195 ENDING TIME OF FILE      24.00


REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
TIMEINTERVAL
     76195       400     76195       500
SCALARS
TGRADBELOW         -.0100
TGRADABOVE          .0039
EXPCLASS          -1.0000
ATMOSPRESS          .9900
RADFACTOR           .0080
CONCWATER      12687.0000
END                 .0000
ENDTIME
```

Exhibit VII-8. Sample Output from the METSCL Program

```
 FILE NAME --METSCALARS         VALUES FOR METEOROLOGICAL SCALARS                              PAGE 01

METEOROLOGICAL SCALARS (VARIABLE UNITS -- CONSULT MANUAL)   START DATE/TIME ,76195  4.00 STOP DATE/TIME 76195  5.00

VARIABLE NAME      VALUE

TGRADBELOW              -.0100

TGRADABOVE               .0039

EXPCLASS              -1.0000

RADFACTOR                .0080

CONCWATER           12687.0000

ATMOSPRESS               .9900

TIME INTERVAL
     76195       500     76195       600
SCALARS
RADFACTOR          .0840
EXPCLASS           .0000
END                .0000
ENDTIME

 FILE NAME --METSCALARS         VALUES FOR METEOROLOGICAL SCALARS                              PAGE 01

METEOROLOGICAL SCALARS (VARIABLE UNITS -- CONSULT MANUAL)   START DATE/TIME ,76195  5.00 STOP DATE/TIME 76195  6.00

VARIABLE NAME      VALUE

TGRADBELOW              -.0100

TGRADABOVE               .0039

EXPCLASS                 .0000

RADFACTOR                .0840

CONCWATER           12687.0000

ATMOSPRESS               .9900

TIME INTERVAL
     76195       600     76195       700
SCALARS
EXPCLASS          1.0000
CONCWATER     12687.0000
RADFACTOR          .1800
END                .0000
ENDTIME
```

Exhibit VII-8 (Concluded)

F. PTSOURCE

The PTSOURCE file contains a set of time-invariant locations of elevated point sources and time-varying emissions fluxes from each source into specific vertical cells. The file can be omitted from a simulation run. The program PTSRCE is used to create the PTSOURCE file. PTSRCE requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-11 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the PTSRCE program.

1. Variables

The output variables for the PTSOURCE file are the species named in the CONTROL packet. Additional user-defined input variables (e.g., "reactive hydrocarbons") can be specified in the UNITS packet. The internal units for the emissions of all species except AEROSOLS are gram-moles per hour (g-mol/hr); for AEROSOLS, the units are grams per hour (g/hr). The standard names for reactive species recognized by the Airshed Simulation Program are listed in Section IX.A. If any of these species does not appear on the PTSOURCE file, the emissions will default to zero. If any additional species appear on PTSOURCE, they will be ignored.

There are five other implicit variables used in the PTSRCE program:

> HEIGHT--stack height
> DIAMETER--stack exit diameter
> STACKTEMP--stack exit temperature
> STACKVEL--stack exit velocity
> FLOWRATE--flow rate.

The internal units for these variables are shown in Table VI-5; input unit conversions for any of these variables can be specified in the UNITS packet without adding to the count of "user-defined variables." Values

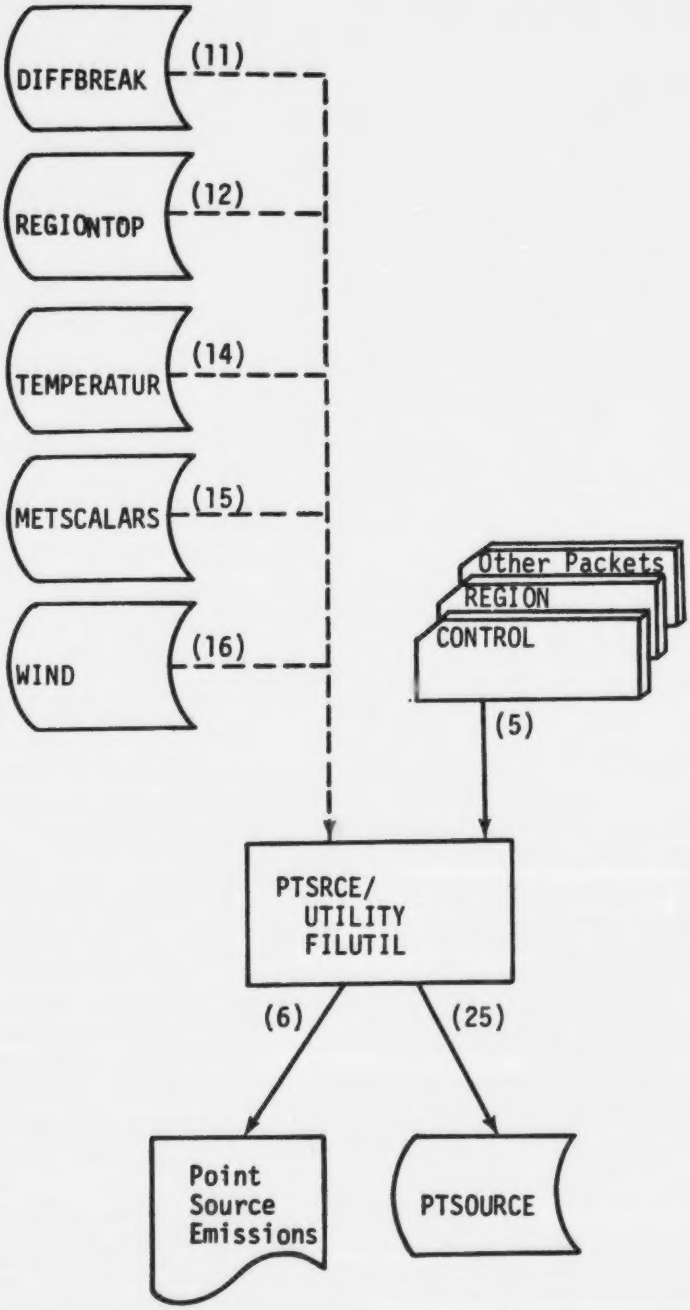

DIFFBREAK
(11)
REGIONTOP
(12)
TEMPERATUR
(14)
METSCALARS
(15)
WIND
(16)
Other Packets
REGION
CONTROL
(5)
PTSRCE/
UTILITY
FILUTIL
(6)
(25)
Point
Source
Emissions
PTSOURCE

Figure VII-11. Information Flow Diagram for the PTSOURCE File

for the first four variables are entered in the POINT SOURCES packet and are considered time-invariant. FLOWRATE values, if specified, appear in the EMISSIONS VALUES packet and are modified, along with species emissions, by the emissions factors.

2. Methods

The methods that can be used to generate the PTSOURCE file are:

> EMVALUES
> EMFACTORS
> SPLIT/COMB
> USER.

These methods are discussed in detail in Section VI.A.6.

Since the PTSOURCE file varies in the vertical direction, a vertical method must also be specified for each output variable in each subregion. The vertical methods that can be used are:

> STACKHGT
> PLUMERISE
> VERTUSER.

These vertical methods are discussed in detail in Section VI.A.7.

3. Time Variation

The time span of the PTSOURCE file must include the entire time span of the simulation runs for which it is to be used. Point source emissions are considered to be constant during each time interval.

4. Packets

Figure VII-12 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the PTSOURCE file:

> CONTROL

- The file name on Card 2 must be PTSOURCE.
- The control variables to be specified on Cards 4 to 8 for PTSOURCE are shown in Table VII-5.
- The number ofspecies must be greater than zero.
- If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.
- The number of point sources defined in the POINT SOURCES packet must be specified.
- The number of point source types must be at least one.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) must specify the maximum number of vertical parameters as applicable.
- The file unit assignment card (No. 8) must specify the DIFFBREAK and REGIONTOP files. In addition, it must specify TEMPERATUR, METSCALARS, and WIND if the vertical method PLUMERISE is selected.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is required; their number must be the same as the entry in the first control parameter on Card 4.

> REGION. This packet must follow the CONTROL packet. The vertical parameters must be provided for the PTSOURCE file.

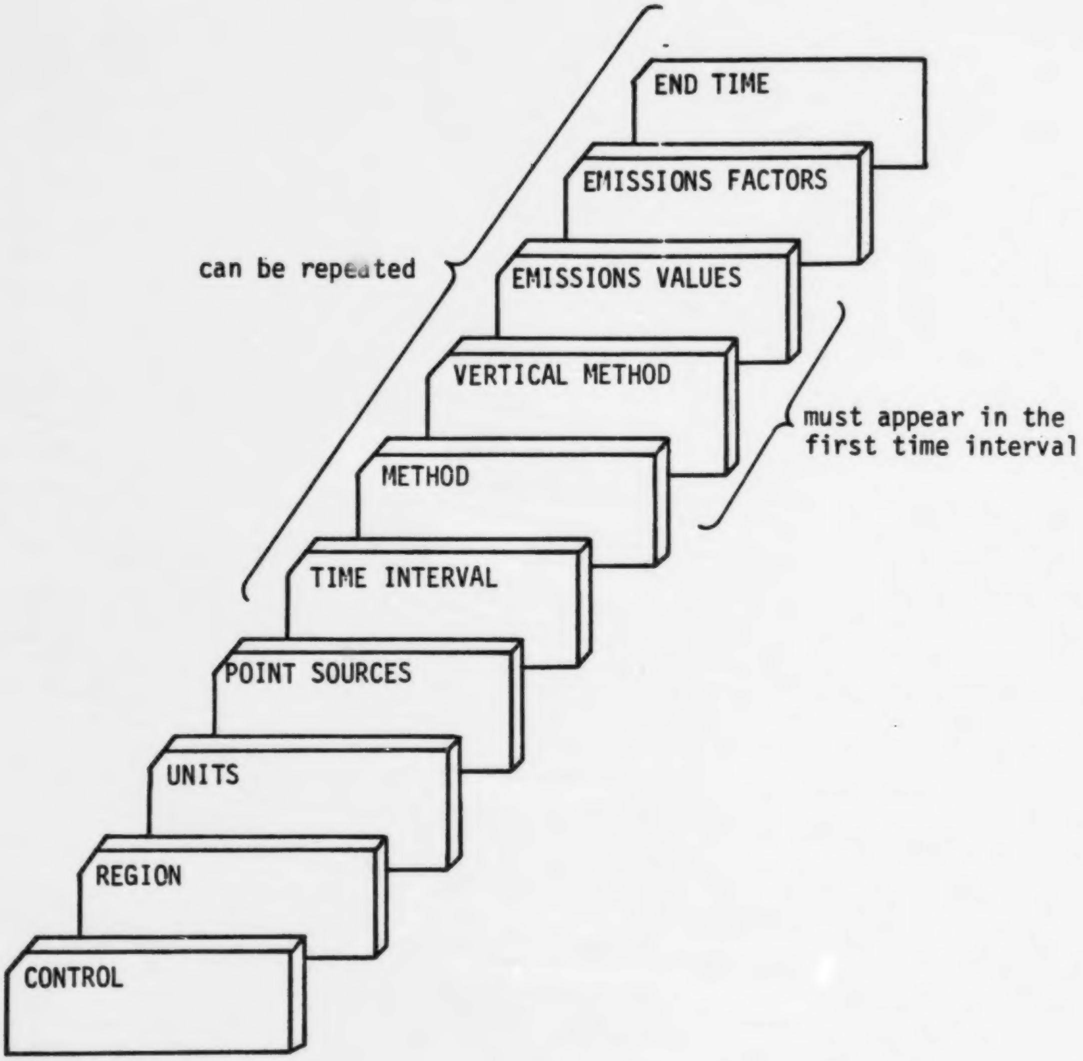

END TIME
EMISSIONS FACTORS
can be repeated
EMISSIONS VALUES
VERTICAL METHOD
must appear in the first time interval
METHOD
TIME INTERVAL
POINT SOURCES
UNITS
REGION
CONTROL

Figure VII-12. Input Card Deck Structure for Preparing the PTSOURCE File

Table VII-5. CONTROL Packet Entries for the PTSOURCE File

Card Number	Entry
4	Number of species
	Number of user-defined variables
	Number of point sources
	Number of point source types
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print point source locations table
	Print regional point source distribution grid
	Print methods table
	Print point source values table
	Spare
7	Number of vertical parameters
	Spare
	Print vertical methods table
	Spare
	Spare
	Spare
8	DIFFBREAK file number
	REGIONTOP file number
	Spare
	TEMPERATUR file number
	METSCALARS file number
	WIND file number

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:
  - Any input variable will be input in other than internal units.
  - Any user-defined variables are specified.
  - COORD or HEIGHT unit conversions are to be used.

  The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> POINT SOURCES. This packet is required. It names the point sources, assigns to each a type and location, and describes certain time-invariant stack properties. The number of point sources specified must equal the number specified in the CONTROL packet. Each point source must be given a type name. Point sources are grouped by type at the time that methods and vertical methods are assigned, and emission factors can be applied by point source type. The number of different types specified must not exceed the maximum defined in the CONTROL packet.

> TIME INTERVAL. One or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> METHOD. A method must be provided for every variable--including user-defined variables--for every point source type in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

- VERTICAL METHOD. A vertical method must be provided for every variable--including user-defined variables--for every point source type in the first time interval. Vertical methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each vertical parameter entry contributes to the overall vertical parameter count; the total must not exceed the maximum specified in the CONTROL packet.
- EMISSIONS VALUES. The first time interval must contain an EMISSIONS VALUES packet. More than one EMISSIONS VALUES packet can appear in any time interval.
- EMISSIONS FACTORS. If the method EMFACTORS is selected in a subsequent time interval, the EMISSIONS FACTORS packet must appear. This packet can be used to multiply all emissions from a given point source or type by a time-varying factor. More than one EMISSIONS FACTORS packet can appear in any time interval.

5. Additional Input Files

The DIFFBREAK and REGIONTOP files must be input to PTSRCE. In addition, if the vertical method PLUMERISE was selected, the TEMPERATUR, METSCALARS, and WIND files must also be input.

6. Examples

Exhibit VII-9 shows a sample input deck for PTSOURCE file generation. The output from a PTSRCE run using that input deck is shown in Exhibit VII-10.

```
CONTROL
PTSOURCE
   POINT SOURCES FOR ST. LOUIS  76195   4X4 GRID
         9         2       217         1        10
        25         0         1
         1         0         0         0         1
                             0
        11        12                  14        15        16
NO
NO2
PAR
OLE
CARB
ARO
SO2
AERS
CO
     76195      0500     76195      2400
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.      50.0      200.
END
UNITS
NO         KG/HR
NO2        KG/HR
PAR
OLE
CARB
ARO
SO2        KG/HR
AERS       KG/HR                                  1.
CO         KG/HR
FLOWRATE   M3/MIN              60.        0.        1.
NOX        KG/HR             1000.                 46.
SOX        KG/HR             1000.                 62.
END
POINT SOURCES
1414400101ST.LOUIS          78900.    32100.
         4                     286
1414400201ST.LOUIS          77713.    26692.
        24                     671
1414400401ST.LOUIS          87700.    23100.
        12                     616
1446800101ST.LOUIS          23710.    53630.
        76                     437
1446800102ST.LOUIS          23750.    53600.
        76                     421
```

Exhibit VII-9. Sample Input Deck for the PTSRCE Program

```
14468001033ST.LOUIS        23770.    53580.
      106                     417
14468002015T.LOUIS        31720.    38880.
        9                     758
14468003075T.LOUIS        20520.    31130.
       72                     438
14468004015T.LOUIS        27330.    52550.
       48                     471
14468004075T.LOUIS        27220.    51850.
       48                     563
14468004095T.LOUIS        27190.    52030.
       33                     755
14468004145T.LOUIS        27180.    52010.
       33                     588
14468004175T.LOUIS        27170.    52310.
       23                     644
14468004215T.LOUIS        27130.    51570.
       45                    1088
14468004225T.LOUIS        26880.    52130.
       23                    1032
14468004235T.LOUIS        27180.    52300.
       15                     921
14468004245T.LOUIS        27020.    52010.
       15                     286
14468004365T.LOUIS        27920.    51120.
       17                     286
14468004645T.LOUIS        26960.    51900.
       52                     574
14468005025T.LOUIS        27770.    50150.
       24                     532
```

•
•
•

Exhibit VII-9 (Continued)

```
•
•
•

1446800304ST.LOUIS      20520.    31070.
        72                 455
1446800303ST.LOUIS      20520.    31050.
        72                 455
1446800603ST.LOUIS      19300.    57400.
         4                 286
1469001005ST.LOUIS      22000.    17700.
         4                 286
END
TIME INTERVAL
     76195       500     76195       600
METHOD
ST.LOUIS  ALL       EMVALUES         0.    50000.
ST.LOUIS  NO        SPLIT/COMB       0.    50000.
NOX             0.9                                        1
ST.LOUIS  NO2       SPLIT/COMB       0.     2000.
NOX             0.1                                        1
ST.LOUIS  SO2       SPLIT/COMB       0.    50000.
SOX             1.0                                        1
END
VERTICAL METHODS
ST.LOUIS  ALL       PLUME RISE       0.0   10000.
END
EMISSIONS VALUES
ALL       ALL            0.0
1414400104AERS            .34
1414400201FLOW RATE     57.77
1414400201NOX            3.12
1414400201SOX             .17
1414400201CO              .85
1414400201AERS            .12
1414400201PAR           29.27
1414400201OLE             .37
1414400201CARB            .37
1414400201ARO             .12
1414400401FLOW RATE     28.32
1414400401NOX           20.97
1414400401CO             2.65
1414400401AERS            .06
1414400401PAR          817.23
```

Exhibit VII-9 (Concluded)

```
CONTROL
PTSOURCE
   POINT SOURCES FOR ST. LOUIS  76195   4X4 GRID
         9          2         217         1         10          0
        25          0           1         0          0          0
         1          0           0         0          1          0
         0          0           0         0          0          0
        11         12           0        14         15         16
NO
NO2
PAR
OLE
CARB
ARO
SO2
AERS
CO
     76195       500     76195       2400
END
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE PTSOURCE

   POINT SOURCES FOR ST. LOUIS  76195   4X4 GRID


REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
KCRNT =    111  NSCLFT = 23390  IN SCRSET
KCRNT =    171  NSCLFT = 23330  IN SCRSET
KCRNT =    341  NSCLFT = 23160  IN SCRSET
KCRNT =    358  NSCLFT = 23143  IN SCRSET
KCRNT =    375  NSCLFT = 23126  IN SCRSET
```

Exhibit VII-10. Sample Output from the PTSRCE Program

```
KCRNT =   392  NSCLFT = 23109  IN SCRSET
KCRNT =   398  NSCLFT = 23103  IN SCRSET
KCRNT =  2568  NSCLFT = 20933  IN SCRSET
KCRNT =  2578  NSCLFT = 20923  IN SCRSET
KCRNT =  2795  NSCLFT = 20706  IN SCRSET
KCRNT =  3012  NSCLFT = 20489  IN SCRSET
KCRNT =  3229  NSCLFT = 20272  IN SCRSET
KCRNT =  5616  NSCLFT = 17885  IN SCRSET
KCRNT =  8003  NSCLFT = 15498  IN SCRSET
KCRNT =  8014  NSCLFT = 15487  IN SCRSET
KCRNT =  8025  NSCLFT = 15476  IN SCRSET
KCRNT =  8036  NSCLFT = 15465  IN SCRSET
KCRNT =  8047  NSCLFT = 15454  IN SCRSET
KCRNT =  8058  NSCLFT = 15443  IN SCRSET
KCRNT =  8158  NSCLFT = 15343  IN SCRSET
KCRNT =  8168  NSCLFT = 15333  IN SCRSET
KCRNT =  8179  NSCLFT = 15322  IN SCRSET
KCRNT =  8190  NSCLFT = 15311  IN SCRSET
KCRNT =  8201  NSCLFT = 15300  IN SCRSET
KCRNT =  8212  NSCLFT = 15289  IN SCRSET
KCRNT =  8223  NSCLFT = 15278  IN SCRSET
KCRNT =  8440  NSCLFT = 15061  IN SCRSET
KCRNT =  8657  NSCLFT = 14844  IN SCRSET
KCRNT =  8874  NSCLFT = 14627  IN SCRSET
KCRNT =  9091  NSCLFT = 14410  IN SCRSET
KCRNT =  9465  NSCLFT = 14036  IN SCRSET
KCRNT =  9839  NSCLFT = 13662  IN SCRSET
KCRNT = 10213  NSCLFT = 13288  IN SCRSET
KCRNT = 11709  NSCLFT = 11792  IN SCRSET
KCRNT = 13205  NSCLFT = 10296  IN SCRSET
KCRNT = 13579  NSCLFT =  9922  IN SCRSET
KCRNT = 13796  NSCLFT =  9705  IN SCRSET
KCRNT = 14013  NSCLFT =  9488  IN SCRSET
KCRNT = 14230  NSCLFT =  9271  IN SCRSET
KCRNT = 14447  NSCLFT =  9054  IN SCRSET
KCPNT = 14664  NSCLFT =  8837  IN SCRSET
KCRNT = 17051  NSCLFT =  6450  IN SCRSET
UNITS
```

Exhibit VII-10 (Continued)

```
                                   UNIT CONVERSION TABLE
VARIABLE NAME        UNIT NAME     MULTIPLICATIVE FACTOR   ADDITIVE FACTOR

   NO                 KG/HR             1000.00000000         -9.00000000        30.00000000
   NO2                KG/HR             1000.00000000         -9.00000000        46.00000000
   PAR                                    -9.00000000         -9.00000000        -9.00000000
   OLE                                    -9.00000000         -9.00000000        -9.00000000
   CARB                                   -9.00000000         -9.00000000        -9.00000000
   ARO                                    -9.00000000         -9.00000000        -9.00000000
   SO2                KG/HR             1000.00000000         -9.00000000        64.00000000
   AERS               KG/HR             1000.00000000         -9.00000000         1.00000000
   CO                 KG/HR             1000.00000000         -9.00000000        28.00000000
   NOX                KG/HR             1000.00000000         -9.00000000        46.00000000
   SOX                KG/HR             1000.00000000         -9.00000000        62.00000000
   COORD                                  -9.00000000         -9.00000000        -9.00000000
   HEIGHT                                 -9.00000000         -9.00000000        -9.00000000
   DIAMETER                               -9.00000000         -9.00000000        -9.00000000
   STACKTEMP                              -9.00000000         -9.00000000        -9.00000000
   STACKVEL                               -9.00000000         -9.00000000        -9.00000000
   FLOWRATE           M3/MIN              60.00000000         -9.00000000         1.00000000
```

Exhibit VII-10 (Continued)

```
POINT SOURCES
TIME INTERVAL
     76195       500     76195       600
METHOD
VERTICAL METHODS
EMISSIONS VALUES
ENDTIME
****** NOTE ****** EMISSIONS FROM POINT SOURCE 1414400104 IN CELL (        25,        13)

ARE OUTSIDE HORIZONTAL DIMENSIONS OF MODEL DOMAIN. EMISSIONS FROM THIS SOURCE HAVE BEEN SET TO ZERO

****** NOTE ****** EMISSIONS FROM POINT SOURCE 1414400201 IN CELL (        25,        11)

ARE OUTSIDE HORIZONTAL DIMENSIONS OF MODEL DOMAIN. EMISSIONS FROM THIS SOURCE HAVE BEEN SET TO ZERO

****** NOTE ****** EMISSIONS FROM POINT SOURCE 1414400401 IN CELL (        27,        10)

ARE OUTSIDE HORIZONTAL DIMENSIONS OF MODEL DOMAIN. EMISSIONS FROM THIS SOURCE HAVE BEEN SET TO ZERO

****** NOTE ****** EMISSIONS FROM POINT SOURCE 1446803301 IN CELL (        21,        15)

ARE OUTSIDE HORIZONTAL DIMENSIONS OF MODEL DOMAIN. EMISSIONS FROM THIS SOURCE HAVE BEEN SET TO ZERO

****** NOTE ****** EMISSIONS FROM POINT SOURCE 1464600101 IN CELL (        18,         1)

ARE OUTSIDE HORIZONTAL DIMENSIONS OF MODEL DOMAIN. EMISSIONS FROM THIS SOURCE HAVE BEEN SET TO ZERO

****** NOTE ****** EMISSIONS FROM POINT SOURCE 1464600103 IN CELL (        18,         1)

ARE OUTSIDE HORIZONTAL DIMENSIONS OF MODEL DOMAIN. EMISSIONS FROM THIS SOURCE HAVE BEEN SET TO ZERO
```

Exhibit VII-10 (Continued)

POINT SOURCE EMISSIONS (GRAM-MOLES/HOUR) SPECIES NO

PT. SOURCE NAME	PT. SOURCE TYPE NAME	X-CELL	Y-CELL	Z-CELL	FLOW RATE (M**3/HOUR)	PLUME HGT. (METERS)	EMS. VALUE (G-MOL/HR)	EMS. FACTOR (G-MOL/HR)	EMS. FLUX
1446800101	ST.LOUIS	11	18	3	224607.	209.2825	.00	-9.00	2778.85
1446800102	ST.LOUIS	11	18	3	143602.	186.3772	.00	-9.00	173.93
1446800103	ST.LOUIS	11	18	3	940271.	310.3101	.00	-9.00	13977.59
1446800201	ST.LOUIS	13	14	1	10610.	37.2358	.00	-9.00	57.72
1446800307	ST.LOUIS	10	12	2	708572.	267.5112	.00	-9.00	8499.52
1446800401	ST.LOUIS	12	18	3	168270.	177.9466	.00	-9.00	3082.70
1446800407	ST.LOUIS	12	17	3	232827.	214.4082	.00	-9.00	655.63
1446800409	ST.LOUIS	12	18	3	93777.	180.0519	.00	-9.00	578.15
1446800414	ST.LOUIS	12	18	2	34609.	106.4060	.00	-9.00	135.20
1469003401	ST.LOUIS	12	12	1	21472.	25.0118	.00	-9.00	19.37
2622800101	ST.LOUIS	6	1	1	7767.	41.9041	.00	-9.00	373.11
2641600101	ST.LOUIS	8	19	4	884461.	391.2513	.00	-9.00	123442.24
2642800301	ST.LOUIS	10	10	1	53908.	157.5535	.00	-9.00	1091.15
2642800302	ST.LOUIS	10	10	1	1274.	77.3614	.00	-9.00	20.35
2642800305	ST.LOUIS	10	10	1	52349.	85.0143	.00	-9.00	795.13
2642800601	ST.LOUIS	9	13	1	28226.	127.1465	.00	-9.00	328.30
2642801201	ST.LOUIS	9	9	2	88058.	216.5848	.00	-9.00	6.46
2642801202	ST.LOUIS	9	9	2	103633.	202.7230	.00	-9.00	6.46
2642801701	ST.LOUIS	10	12	1	26015.	104.6543	.00	-9.00	355.89
2642801704	ST.LOUIS	10	12	1	797.	40.1493	.00	-9.00	9.98
2642801705	ST.LOUIS	10	12	1	21491.	49.4752	.00	-9.00	444.13
2642802302	ST.LOUIS	10	11	1	41191.	104.3999	.00	-9.00	854.02
2642802401	ST.LOUIS	10	13	2	177407.	291.4135	.00	-9.00	393.07
2642802501	ST.LOUIS	9	10	2	177407.	291.7539	.00	-9.00	393.07
2642803801	ST.LOUIS	10	12	1	61006.	139.7895	.00	-9.00	722.15
2642804001	ST.LOUIS	9	11	1	9312.	85.9915	.00	-9.00	196.24
2642805601	ST.LOUIS	9	12	1	1099.	16.8529	.00	-9.00	42.26
2642805702	ST.LOUIS	10	13	1	16990.	57.9199	.00	-9.00	52.63
2642805801	ST.LOUIS	10	12	1	43367.	91.3986	.00	-9.00	498.52
2642805901	ST.LOUIS	9	11	1	16990.	65.4218	.00	-9.00	.98
2642806001	ST.LOUIS	9	13	1	16990.	65.0096	.00	-9.00	1.96
2643000101	ST.LOUIS	7	8	3	407762.	258.4892	.00	-9.00	2244.33
2643000208	ST.LOUIS	4	9	1	4499.	57.4342	.00	-9.00	368.80
2643000701	ST.LOUIS	6	15	1	5097.	28.8824	.00	-9.00	216.39
2643000704	ST.LOUIS	6	15	1	7287.	42.0511	.00	-9.00	102.91
2643000708	ST.LOUIS	7	15	1	3309.	34.5166	.00	-9.00	85.30
2643000801	ST.LOUIS	9	14	3	679603.	299.2691	.00	-9.00	4935.72
2643000901	ST.LOUIS	9	9	1	57008.	88.8184	.00	-9.00	620.02
2643000903	ST.LOUIS	9	9	1	71429.	93.7199	.00	-9.00	1331.02
2643000905	ST.LOUIS	9	9	1	23143.	54.6988	.00	-9.00	126.78
2643000910	ST.LOUIS	9	9	1	47572.	75.3069	.00	-9.00	88.43
2643000911	ST.LOUIS	9	9	1	110435.	82.1603	.00	-9.00	88.43
2643000913	ST.LOUIS	9	9	1	118931.	96.3039	.00	-9.00	88.43
2643001001	ST.LOUIS	7	5	3	244627.	205.0220	.00	-9.00	11451.13
2643001003	ST.LOUIS	7	5	3	832438.	311.3381	.00	-9.00	32980.50
2643001401	ST.LOUIS	8	8	1	4078.	78.8097	.00	-9.00	37.96
2643001601	ST.LOUIS	8	12	1	8860.	85.0452	.00	-9.00	156.33
2643003101	ST.LOUIS	4	9	1	0.	17.9998	.00	-9.00	101.74

Exhibit VII-10 (Continued)

```
                                                                                             PAGE  1
FILE NAME -- PTSOURCE         POINT SOURCES FOR ST. LOUIS  76195   4X4 GRID
POINT SOURCE EMISSIONS (GRAM-MOLES/HOUR) SPECIES  NO        VERT.  LEVEL 0 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        1         2         3         4         5         6         7         8         9        10        11        12
   22           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
   21           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
   20           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
   19           .00       .00       .00       .00       .00       .00       .00 123442.24       .00     21.33       .00       .00
   18           .00       .00       .00       .00       .00       .00       .00       .00       .00    639.59  22346.61   4501.76
   17           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00   5216.28
   16           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
   15           .00       .00       .00       .00       .00    319.30     85.30       .00       .00       .00       .00       .00
   14           .00       .00       .00       .00       .00       .00       .00       .00   4935.72       .00     19.76       .00
   13           .00       .00       .00       .00       .00       .00       .00       .00    330.26    445.70   6952.89       .00
   12           .00       .00       .00       .00       .00       .00       .00    156.33     42.26  10530.20    292.11     19.37
   11           .00       .00       .00       .00       .00       .00       .00       .00    197.22    854.02   1329.46       .00
   10           .00       .00       .00       .00       .00       .00       .00       .00    393.07   1906.63   2464.83      9.78
    9           .00       .00       .00    470.54       .00       .00       .00       .00   2356.04       .00       .00       .00
    8           .00       .00       .00       .00       .00       .00   2244.33     37.96       .00       .00       .00       .00
    7           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
    6           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
    5           .00       .00       .00       .00       .00       .00  44431.63       .00       .00       .00       .00       .00
    4           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
    3           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
    2           .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00       .00
    1           .00       .00       .00       .00       .00    373.11       .00       .00       .00       .00       .00       .00
```

Exhibit VII-10 (Continued)

```
                                                                                                          PAGE  2
FILE NAME -- PTSOURCE          POINT SOURCES FOR ST. LOUIS  76195   4X4 GRID
POINT SOURCE EMISSIONS (GRAM-MOLES/HOUR) SPECIES  NO        VERT.  LEVEL 0 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        13          14          15          16          17
     22          .00         .00         .00         .00         .00
     21          .00         .00         .00         .00         .00
     20          .00         .00         .00         .00         .00
     19          .00         .00         .00         .00         .00
     18          .00         .00         .00         .00         .00
     17      1761.46         .00         .00         .00         .00
     16          .00         .00         .00         .00         .00
     15          .00         .00         .00         .00         .00
     14        57.72         .00         .00         .00         .00
     13          .00         .00         .00         .00         .00
     12          .00         .00         .00         .00         .00
     11          .00         .00         .00         .00         .00
     10          .00         .00         .00         .00         .00
      9          .00         .00         .00         .00      191.74
      8          .00       63.39       23.48         .00         .00
      7          .00         .00         .00         .00         .00
      6          .00         .00         .00         .00         .00
      5          .00         .00         .00         .00         .00
      4          .00         .00         .00         .00         .00
      3          .00         .00         .00         .00         .00
      2          .00         .00         .00         .00         .00
      1          .00         .00         .00         .00         .00
```

Exhibit VII-10 (Concluded)

G. REGIONTOP

The REGIONTOP file contains time-varying two-dimensional matrices of region top heights. The region top height can be linked to the diffusion break or can be independently specified. The program REGNTP is used to create the REGIONTOP file. REGNTP requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-13 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the REGNTP program.

1. Variables

The output variable for the REGIONTOP file is also named REGIONTOP. This is an "implicit output variable" and need not be referred to anywhere in the CONTROL packet. The internal units for REGIONTOP are meters (m). If the input values for this variable are to be in any other units, REGIONTOP must be specified in the UNITS packet.

2. Methods

The methods that can be used to generate the REGIONTOP file are:

- > CONSTANT
- > GRID VALUE
- > STATINTERP
- > POISSON
- > FIXDHEIGHT
- > SAMEHEIGHT
- > E-WINTERP
- > N-SINTERP
- > USER.

These methods are discussed in detail in Section VI.A.6.

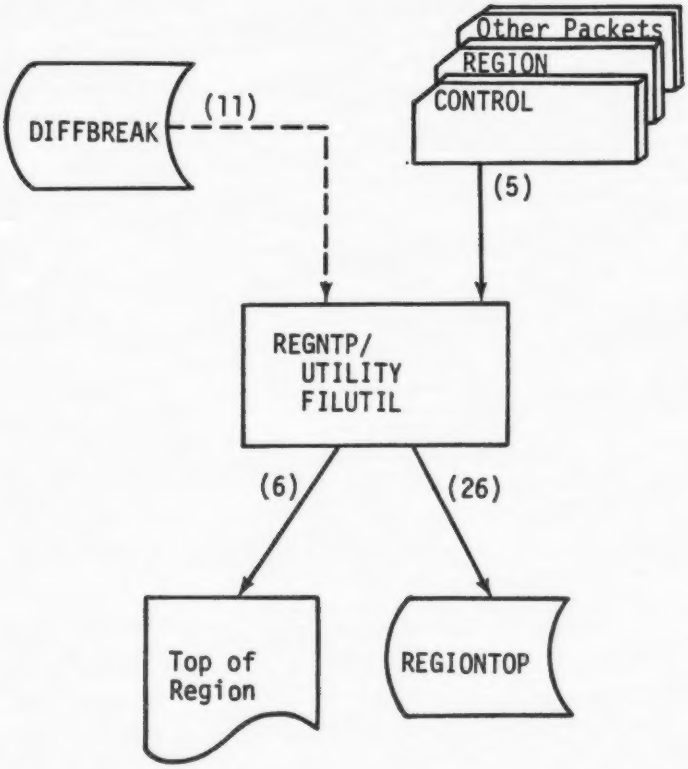

Other Packets
REGION
CONTROL
DIFFBREAK
(11)
(5)
REGNTP/
UTILITY
FILUTIL
(6)
(26)
Top of Region
REGIONTOP

Figure VII-13. Information Flow Diagram for the REGIONTOP File

3. Time Variation

The top of the region values on the REGIONTOP file are considered to apply at the beginning of the time interval. Because the Airshed Simulation Program calculates region top values continuously over time by linear interpolation, it also requires values at the end of the time interval. These are read by the program as the values at the beginning of the next time interval. Thus, the last time interval on the file must begin at or after the ending simulation time. For example, if a simulation is to be made from 0500-1700 and region top values are input hourly, the values used between 500 and 600 are calculated by interpolating between values input for the 0500-0600 time interval and those input for the 0600-0700 time interval. Similarly, to calculate values between 1600 and 1700, the simulation program requires values for the interval 1600-1700, and another set for an interval beginning at 1700.

4. Packets

Figure VII-14 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Sections VI.B. Following are special input packet considerations for the REGIONTOP file:

- > CONTROL
  - The file name on Card 2 must be REGIONTOP.
  - The control variables to be specified on Cards 4 to 8 for REGIONTOP are shown in Table VII-6.
  - The number of species should be zero.
  - If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.
  - If data from measuring stations are to be used (methods STATINTERP or POISSON), the maximum number of such stations must be given.
  - The number of subregions must be at least one.

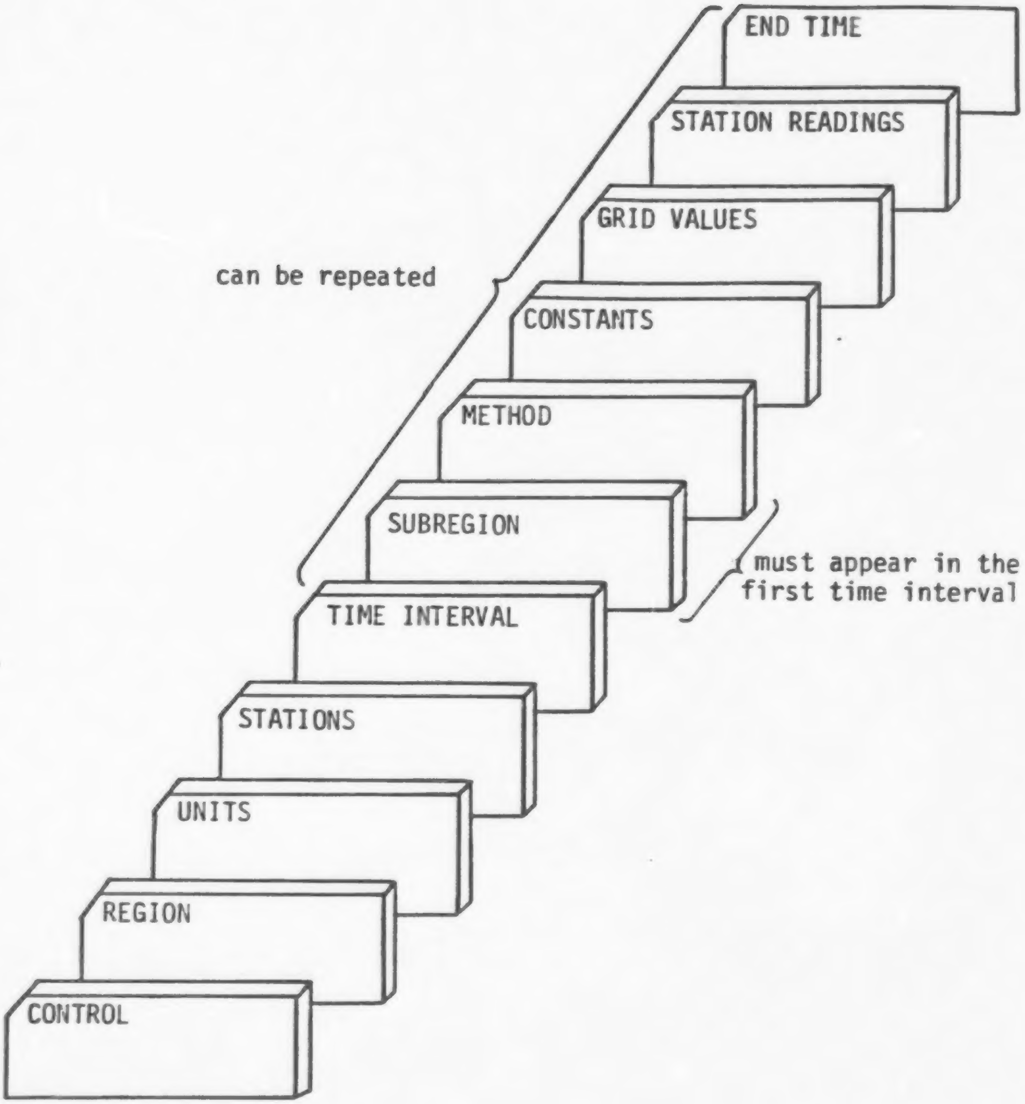

END TIME
STATION READINGS
GRID VALUES
can be repeated
CONSTANTS
METHOD
SUBREGION
must appear in the first time interval
TIME INTERVAL
STATIONS
UNITS
REGION
CONTROL

Figure VII-14. Input Card Deck Structure for Preparing the REGIONTOP File

Table VII-6. CONTROL Packet Entries for the REGIONTOP File

Card Number	Entry
4	Number of species (=0)
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
8	DIFFBREAK file unit number
	Spare
	Spare
	Spare
	Spare
	Spare

  - The maximum number of parameters must be sufficient to include all specifications of all parameters.
  - The vertical controls card (No. 7) should be left blank.
  - The file unit assignment card (No. 8) must specify DIFFBREAK if the method FIXDHEIGHT or SAMEHEIGHT is selected. Otherwise, it should be left blank.
  - The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
  - A set of output species names is not required; if they are present, their number must be the same as the entry in the first control parameter on Card 4, but they will be ignored by the program.
- REGION. This packet must follow the CONTROL packet. The vertical parameters must be provided if FIXDHEIGHT or SAMEHEIGHT is selected. Otherwise, they will be ignored.
- UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:
  - Any input variable will be input in other than internal units.
  - Any user-defined variables are specified.
  - COORD or HEIGHT unit conversions are to be used.

  The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.
- STATIONS. This packet is required if either of the methods STATINTERP or POISSON is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.
- TIME INTERVAL. Two or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. The last time interval must begin at or after the ending time of any simulation run. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following

packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.*

> SUBREGION. The first time interval must contain a SUBREGION packet; the inclusion of this packet in other time intervals is optional. The number of subregions must not exceed the maximum specified in the CONTROL packet.

> METHOD. A method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.

> GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, the first time interval must contain a GRID VALUES packet. More than one GRID VALUES packet can appear in any time interval.

> STATION READINGS. If either the POISSON or STATINTERP method is assigned to any variable in the METHOD packet, the first time interval must contain a STATION READINGS packet. More than one STATION READINGS packet can appear in any time interval.

5. Additional Input Files

If the method FIXDHEIGHT or SAMEHEIGHT was selected, the DIFFBREAK file must be input to REGNTP. Otherwise no additional input files are required.

---

* If FIXDHEIGHT or SAMEHEIGHT is used, the time intervals specified here must be exactly the same as those on the DIFFBREAK file; after the first time interval, subsequent packets may contain no other packets.

6. Examples

Exhibit VII-11 shows a sample input deck for REGIONTOP file generation. The output from a REGNTP run using that input deck is shown in Exhibit VII-12.

```
CONTROL
REGIONTOP
   HEIGHT OF THE TOP OF THE MODELING REGION
                                           1         5
         26         1         1
          1         1         1          1         0

         11
      76195       500     76196         10
END
REGION
   725000.  4252000.         15
   -19000.   -16000.
     4000.     4000.
         17        22         4
          2         2         0.        50.       200.
END
TIME INTERVAL
      76195       500     76195        600
SUBREGION
A                   1         1         -1
END
METHOD
A         REGIONTOP FIXDHEIGHT    500.    2038.           1
UPCELLHT       200.
END
ENDTIME
TIME INTERVAL
      76195       600     76195        700
ENDTIME
TIME INTERVAL
      76195       700     76195        800
ENDTIME
TIME INTERVAL
      76195       800     76195        900
ENDTIME
TIME INTERVAL
      76195       900     76195       1000
ENDTIME
```

Exhibit VII-11.   Sample Input Deck from the REGNTP Program

```
TIME INTERVAL
     76195     1000     76195     1100
ENDTIME
TIME INTERVAL
     76195     1100     76195     1200
ENDTIME
TIME INTERVAL
     76195     1200     76195     1300
ENDTIME
TIME INTERVAL
     76195     1300     76195     1400
ENDTIME
TIME INTERVAL
     76195     1400     76195     1500
ENDTIME
TIME INTERVAL

     76195     1500     76195     1600
ENDTIME
TIME INTERVAL
     76195     1600     76195     1700
ENDTIME
TIME INTERVAL
     76195     1700     76195     1800
ENDTIME
TIME INTERVAL
     76195     1800     76195     1900
ENDTIME
TIME INTERVAL
     76195     1900     76195     2000
ENDTIME
TIME INTERVAL
     76195     2000     76195     2100
ENDTIME
TIME INTERVAL
     76195     2100     76195     2200
ENDTIME
TIME INTERVAL
     76195     2200     76195     2300
ENDTIME
TIME INTERVAL
     76195     2300     76195     2400
ENDTIME
TIME INTERVAL
     76195     2400     76196       10
ENDTIME
```

Exhibit VII-11 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE REGIONTOP

   HEIGHT OF THE TOP OF THE MODELING REGION

NUMBER OF STATIONS =          0

NUMBER OF SUBREGIONS =          1

NUMBER OF METHOD PARAMETERS =          5

PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER        26

INPUT DATA FOR DIFFUSION BREAK WILL BE OBTAINED FROM FILE NUMBER        11

INPUT CARDS WILL BE PRINTED

OUTPUT GRID WILL BE PRINTED

UNIT TABLE WILL BE PRINTED

STATION LOCATIONS WILL BE PRINTED

SUBREGION GRID WILL BE PRINTED

METHOD TABLE WILL BE PRINTED

STATION VALUES WILL NOT BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       5.00

ENDING DATE OF FILE      76196 ENDING TIME OF FILE       .17


REGION
   725000.  4252000.       15
   -19000.   -16000.
   4000.00   4000.00
        17        22        4
         2         2      .00     50.00    200.00
END
```

Exhibit VII-12.   Sample Output from the REGNTP Program

```
FILE NAME -- REGIONTOP          HEIGHT OF THE TOP OF THE MODELING REGION
                                                                                                            PAGE  1
REGION TOPVALUES (IN METERS ABOVE GROUND LEVEL)                VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        1         2         3         4         5         6         7         8         9        10        11        12
    22      502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000
    21      502.0000  504.0061  505.9784  507.8764  509.6442  511.2035  512.4517  513.2621  513.4869  512.9678  511.5785  509.4017
    20      502.0000  506.0492  510.0391  513.8977  517.5229  520.7653  523.4199  525.2271  525.8663  524.9496  522.0040  516.6038
    19      502.0000  508.1576  514.2490  520.1900  525.8482  531.0156  535.3871  538.5582  540.0230  539.1342  534.8865  524.9782
    18      502.0000  510.3394  518.6380  526.8301  534.7796  542.2370  548.8003  553.8979  556.8324  556.8625  553.3217  545.7940
    17      502.0000  512.5715  523.1758  533.8129  544.3856  554.6312  564.0430  571.8205  576.9206  578.3270  575.4780  568.5566
    16      502.0000  514.7858  527.7453  541.0099  554.5890  568.2632  581.4332  592.9575  601.1329  604.1504  601.2368  592.7235
    15      502.0000  516.8553  532.1119  548.1159  565.0816  582.9509  601.1351  618.0985  630.9451  635.9049  631.8983  619.3304
    14      502.0000  518.5852  535.8983  554.5894  575.1980  598.0348  622.8621  648.0858  669.0660  676.4828  670.2190  649.5590
    13      502.0000  519.7123  538.5788  559.6205  583.7796  611.9917  645.0963  683.0558  721.0929  730.4662  721.8958  683.8507
    12      502.0000  519.9191  539.5127  562.1920  589.1754  622.0373  663.4087  718.6224  802.0000  802.0000  802.0000  718.1304
    11      502.0000  518.8524  537.9964  561.3214  589.7096  624.6137  668.7601  726.5473  802.0000  802.0000  802.0000  724.6042
    10      502.0000  516.1240  533.1719  556.4365  584.8351  618.9656  661.2449  717.1955  802.0000  802.0000  802.0000  713.3499
     9      502.0000  511.3740  523.2244  547.5830  575.3284  606.0785  640.6791  679.2575  717.1860  725.2433  714.3020  672.3603
     8      502.0000  505.3165  502.0000  536.5030  563.7951  590.0691  616.5829  642.1357  662.1583  667.2108  657.2377  631.7732
     7      502.0000  507.2511  514.7118  533.6508  554.0439  574.3307  593.7312  610.6377  622.0515  624.0679  615.5090  596.6989
     6      502.0000  508.3177  517.0373  530.1234  544.9114  559.7828  573.5247  584.6783  591.3240  591.4567  583.9997  568.4714
     5      502.0000  508.1039  515.7802  525.3862  535.9775  546.5089  555.9673  563.2427  567.1079  566.4374  560.5847  549.4631
     4      502.0000  507.0870  513.0524  519.9097  527.2197  534.3517  540.6021  545.2149  547.4289  546.6159  542.4751  535.1894
     3      502.0000  505.6063  509.6386  514.0663  518.6635  523.0710  526.8604  529.5737  530.7749  530.1351  527.5416  523.2044
     2      502.0000  503.8637  505.8902  508.0631  510.2833  512.3872  514.1739  515.4294  515.9563  515.6151  514.3737  512.3549
     1      502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000  502.0000
```

Exhibit VII-12 (Continued)

```
FILE NAME -- REGIONTOP        HEIGHT OF THE TOP OF THE MODELING REGION                                        PAGE  2
REGION TOPVALUES (IN METERS ABOVE GROUND LEVEL)          VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        13        14        15        16        17
     22    502.0000  502.0000  502.0000  502.0000  502.0000
     21    507.2683  507.4373  507.3662  505.8242  502.0000
     20    509.6837  511.9638  512.2625  509.0659  502.0000
     19    502.0000  516.8008  518.0606  512.6005  502.0000
     18    535.3789  532.9462  527.3580  517.1122  502.0000
     17    558.9566  549.4731  537.5922  521.9777  502.0000
     16    580.1956  565.2262  547.5758  526.6674  502.0000
     15    601.3668  580.3163  556.8746  530.8992  502.0000
     14    623.0223  594.5563  565.1207  534.4611  502.0000
     13    644.1440  606.8965  571.6151  537.0459  502.0000
     12    660.6950  614.9730  575.1758  538.1938  502.0000
     11    663.9149  615.4856  574.4594  537.4240  502.0000
     10    653.7866  607.5854  568.9463  534.5254  502.0000
      9    629.6791  591.6240  558.8958  529.6244  502.0000
      8    600.6825  570.1863  545.3731  523.1938  502.0000
      7    571.0517  543.1141  529.3504  515.9792  502.0000
      6    543.7772  502.0000  513.1119  509.5702  502.0000
      5    533.6663  515.8389  511.6856  507.3430  502.0000
      4    523.6634  516.0918  510.5570  506.2150  502.0000
      3    517.7668  512.3746  508.3042  505.0166  502.0000
      2    509.8677  507.3805  505.3094  503.5776  502.0000
      1    502.0000  502.0000  502.0000  502.0000  502.0000
 TIME INTERVAL
    76195       600     76195       700
 ENDTIME
```

Exhibit VII-12 (Concluded)

H. ROADWAY (Not recommended for use at this time)

The ROADWAY file contains time-varying matrices of emission fluxes along roadways and a descriptive parameter for automobile traffic. The ROADWAY file can be omitted from a simulation run if surface layer microscale calculations are not to be performed. At present, there is no general purpose program for creating the ROADWAY file because its generation is highly dependent on the form of the traffic data available. There is a program structure, similar to that of the other data preparation programs, that includes the reading of control packets, unit conversions, and writing the proper output records. This program can be tailored to particular input requirements as necessary. The skeleton program is named ROADWY. It requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-15 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the card input to the ROADWY program.

1. Variables

The output variables for the ROADWAY file are the species named in the CONTROL packet and the parameter CARM, which is to be calculated from the traffic data. Additional user-defined input variables (e.g. "reactive hydrocarbons") can be specified in the UNITS packet. The internal units for the roadway emissions of all species except AEROSOLS are gram-moles per hour (g-mol/hr); for AEROSOLS, the units are grams per hour (g/hr). The internal units for CARM are meters per hour (m/hr). The standard names for reactive species recognized by the Airshed Simulation Program are listed in Chapter IX. If any of these species does not appear on the ROADWAY file, the roadway emissions will default to zero. If any additional species appear on ROADWAY, they will be ignored.

2. Methods

The methods that can be used to generate the ROADWAY file are:

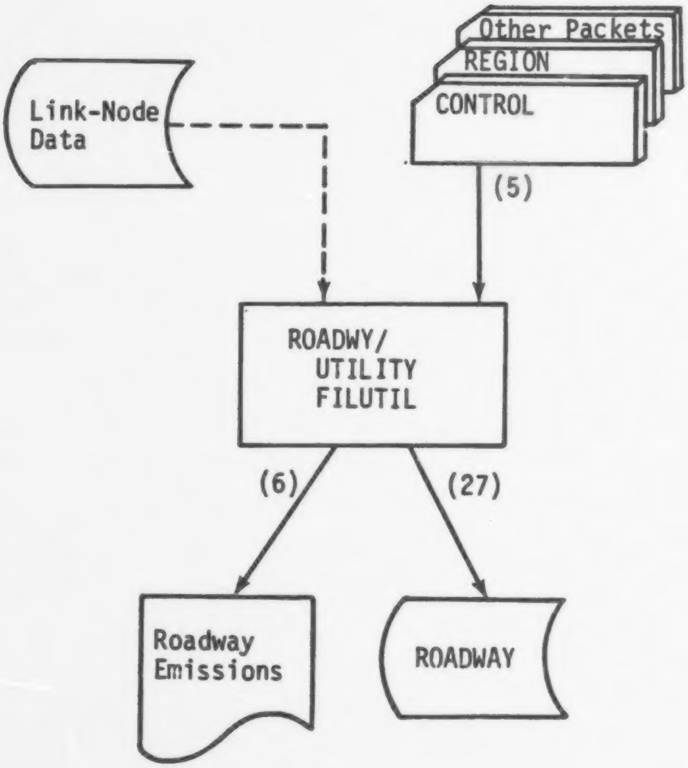

Other Packets
REGION
CONTROL
Link-Node Data
(5)
ROADWY/ UTILITY FILUTIL
(6)
(27)
Roadway Emissions
ROADWAY

Figure VII-15. Information Flow Diagram for the ROADWAY File

> CONSTANT
> ROADVALUE
> SPLIT/COMB
> USER.

The methods ROADVALUE and USER have not been defined. The actual methods for generating output values from input traffic data must be written for each new application.

3. Time Variation

The time span of the ROADWAY file must include the entire time span of the simulation runs for which it is to be used. Roadway emissions and the parameter CARM are considered to be constant during each time interval.

4. Packets

The packets to be used for ROADWY will depend on the particular version that is developed for a given set of traffic data. Information on control parameters, definition of link-node data, units, time intervals, computation methods, and data entry will have to be provided when the program has been implemented. Figure VII-16 shows a possible input structure in terms of the packets to be used.

5. Additional Input Files

In general, a traffic data file in link-node form must be provided.

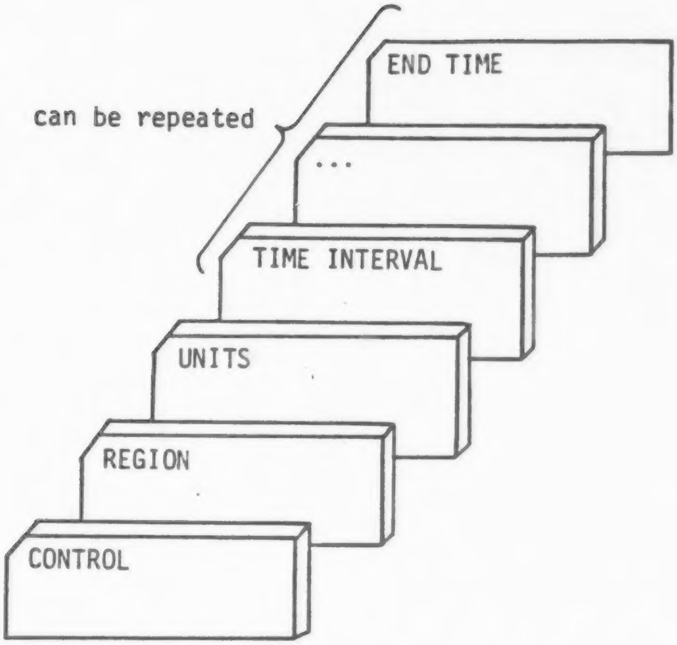

can be repeated
END TIME
...
TIME INTERVAL
UNITS
REGION
CONTROL

Figure VII-16. A Possible Input Card Deck Structure for Preparing the ROADWAY File

I. TEMPERATUR

The TEMPERATUR file contains time-varying matrices of temperatures at ground level. If it is omitted from a simulation run, temperature-dependent calculations will not be performed (see Section IX.B). The program TMPRTR is used to create the TEMPERATUR file. TMPRTR requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-17 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the TMPRTR program.

1. Variables

The output variable for the TEMPERATUR file is also named TEMPERATUR. This is an "implicit output variable" and need not be referred to anywhere in the CONTROL packet. The internal units for TEMPERATUR are °K. If the input values for this variable are to be in any other units, TEMPERATUR must be specified in the UNITS packet..

2. Methods

The methods that can be used to generate the TEMPERATUR file are:

> CONSTANT
> GRID VALUE
> STATINTERP
> POISSON
> E-WINTERP
> N-SINTERP
> USER.

These methods are discussed in detail in Section VI.A.6.

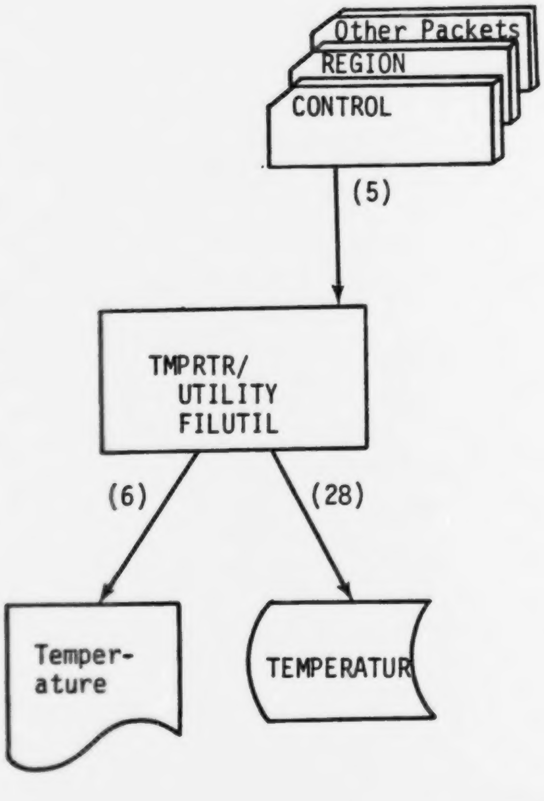

Other Packets
REGION
CONTROL
(5)
TMPRTR/
UTILITY
FILUTIL
(6)
(28)
Temper-
ature
TEMPERATUR

Figure VII-17. Information Flow Diagram for the TEMPERATUR File

3. Time Variation

The time span of the TEMPERATUR file must include the entire time span of the simulation runs for which it is to be used. Ground-level temperatures are considered to be constant during each time interval.

4. Packets

Figure VII-18 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the TEMPERATUR file:

> CONTROL
- The file name on Card 2 must be TEMPERATUR.
- The control variables to be specified on Cards 4 to 8 for TEMPERATUR are shown in Table VII-7.
- The number of species should be zero.
- If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.
- If data from measuring stations are to be used (methods STATINTERP or POISSON), the maximum number of such stations must be given.
- The number of subregions must be at least one.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) should be left blank.
- The file unit assignment card (No. 8) should be left blank.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.

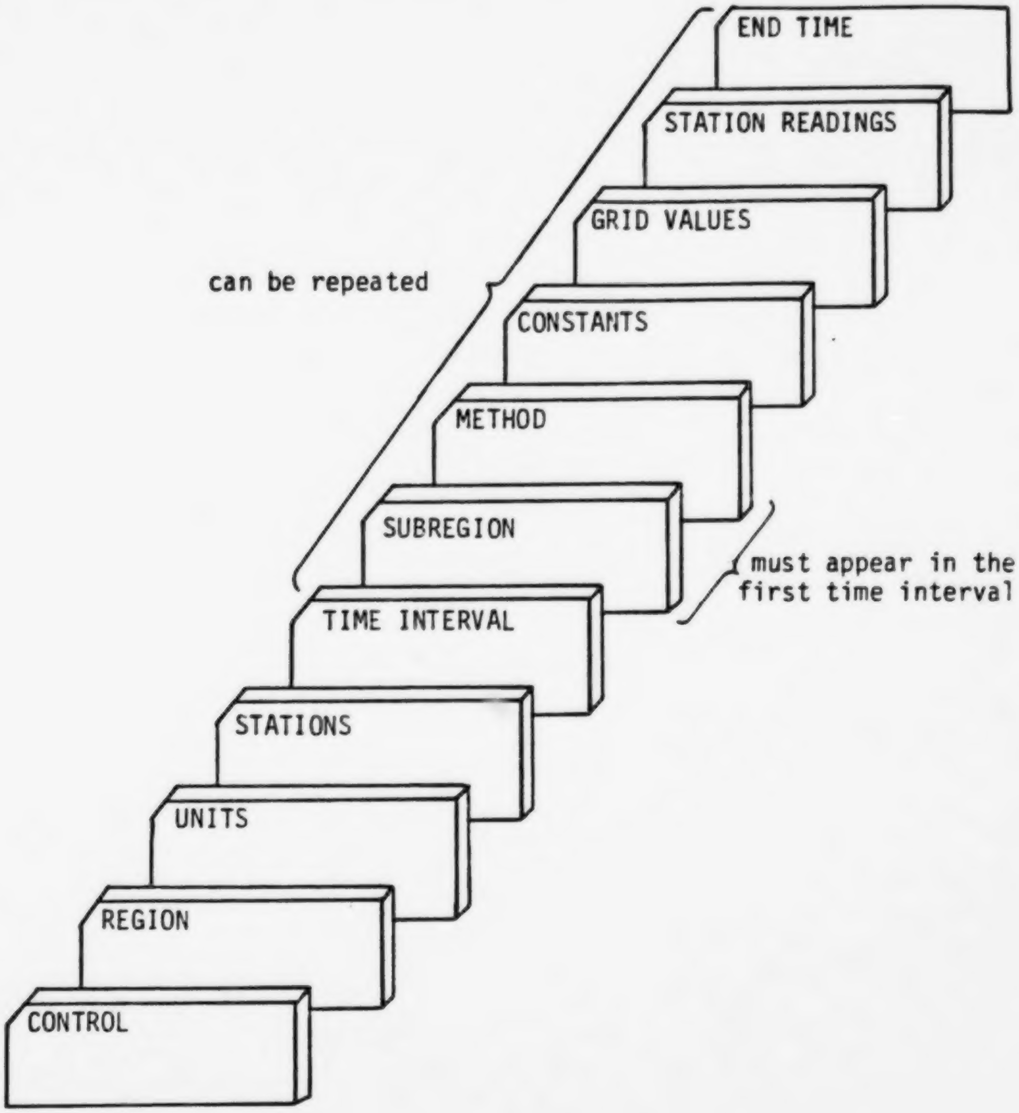

END TIME
STATION READINGS
GRID VALUES
can be repeated
CONSTANTS
METHOD
SUBREGION
must appear in the first time interval
TIME INTERVAL
STATIONS
UNITS
REGION
CONTROL

Figure VII-18. Input Card Deck Structure for Preparing the TEMPERATUR File

Table VII-7. CONTROL Packet Entries for the TEMPERATUR File

Card Number	Entry
4	Number of species (=0)
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
8	Spare
	Spare
	Spare
	Spare
	Spare
	Spare

- A set of output species names is not required; if they are present, their number must be the same as the entry in the first control parameter on Card 4, but they will be ignored by the program.

> REGION. This packet must follow the CONTROL packet. The vertical parameters will be ignored for the TEMPERATUR file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:

- Any input variable will be input in other than internal units.
- Any user-defined variables are specified.
- COORD or HEIGHT unit conversions are to be used.

The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> STATIONS. This packet is required if either of the methods STATINTERP or POISSON is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.

> TIME INTERVAL. One or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> SUBREGION. The first time interval must contain a SUBREGION packet; the inclusion of this packet in other time intervals is optional. The number of subregions must not exceed the maximum specified in the CONTROL packet.

> METHOD. A method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter

entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.

> GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, the first time interval must contain a GRID VALUES packet. More than one GRID VALUES packet can appear in any time interval.

> STATION READINGS. If either the POISSON or STATINTERP method is assigned to any variable in the METHOD packet, the first time interval must contain a STATION READINGS packet. More than one STATION READINGS packet can appear in any time interval.

5. Additional Input Files

No additional input files are required.

6. Examples

Exhibit VII-13 shows a sample input deck for TEMPERATUR file generation. The output from a TMPRTR run using that input deck is shown in Exhibit VII-14.

```
CONTROL
TEMPERATURE
   TEMPERATURE FIELD FOR ST. LOUIS  DAY 195
         0         0        25         1        10
        28         1         1



     76195       500     76195      2400
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2       0.0       50.      200.
END
UNITS
TEMPERATURDEGREES C         1.      273.        1.
END
```

Exhibit VII-13. Sample Input Deck for the TMPRTR Program

```
STATIONS
          101    19183.    27862.        10.
          102    17518.    34045.        10.
          103    22588.    30467.        10.
          104    22312.    25304.        10.
          105    18706.    24453.        10.
          106    13660.    25566.        10.
          107    15179.    30610.        10.
          108    23407.    39102.        10.
          109    30802.    27836.        10.
          110    22209.    20826.        10.
          111    13812.    20479.        10.
          112     8938.    28913.        10.
          113    12738.    37820.        10.
          114    19320.    45456.        10.
          115    32111.    45799.        10.
          116    37777.    38083.        10.
          117    35560.    20818.        10.
          118    18065.    11256.        10.
          119     4759.    18547.        10.
          120    -1921.    33909.        10.
          121     7414.    50376.        10.
          122    16631.    77223.        10.
          123    52320.    34378.        10.
          124    24275.   -15463.        10.
          125   -27555.    30240.        10.
 END
 TIME INTERVAL
      76195       500     76195        600
 SUBREGION
 A                  1         1         -1
 END
 METHOD
 A       TEMPERATURPOISSON             1.        50.        3
 MAXITER       100

 ERRORTOL      0.05
 OMEGA          1.4
 END
```

Exhibit VII-13 (Continued)

```
STATION READINGS
 101       TEMPERATUR       22.4
 102       TEMPERATUR       21.9
 103       TEMPERATUR       21.7
 104       TEMPERATUR       21.4
 105       TEMPERATUR       21.8
 106       TEMPERATUR       22.2
 107       TEMPERATUR       22.5
 108       TEMPERATUR       21.3
 109       TEMPERATUR       21.4
 110       TEMPERATUR       21.3
 111       TEMPERATUR       21.3
 112       TEMPERATUR       22.1
 113       TEMPERATUR       21.4
 114       TEMPERATUR       21.2
 115       TEMPERATUR       21.7
 116       TEMPERATUR       20.3
 117       TEMPERATUR       20.4
 118       TEMPERATUR       21.2
 119       TEMPERATUR       21.6
 120       TEMPERATUR       22.3
 121       TEMPERATUR       21.4
 122       TEMPERATUR       20.0
 123       TEMPERATUR       20.5
 124       TEMPERATUR       19.8
 125       TEMPERATUR       21.4
END
```

Exhibit VII-13 (Continued)

```
STATION READINGS                                        TEMP FOR  500
 101       TEMPERATUR      22.0
 102       TEMPERATUR      21.3
 103       TEMPERATUR      20.3
 104       TEMPERATUR      20.8
 105       TEMPERATUR      21.8
 106       TEMPERATUR      22.2
 107       TEMPERATUR      22.0
 108       TEMPERATUR      20.4
 109       TEMPERATUR      20.0
 110       TEMPERATUR      20.2
 111       TEMPERATUR      21.2
 112       TEMPERATUR      21.8
 113       TEMPERATUR      20.9
 114       TEMPERATUR      20.0
 115       TEMPERATUR      20.3
 116       TEMPERATUR      19.4
 117       TEMPERATUR      19.6
 118       TEMPERATUR      20.0
 119       TEMPERATUR      21.1
 120       TEMPERATUR      21.9
 121       TEMPERATUR      20.4
 122       TEMPERATUR      19.5
 123       TEMPERATUR      19.1
 124       TEMPERATUR      19.1
 125       TEMPERATUR      21.2
END
ENDTIME
TIME INTERVAL
     76195       600     76195       700
                                                        TEMP FOR  600
```

Exhibit VII-13 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE TEMPERATUR

   TEMPERATURE FIELD FOR ST. LOUIS  DAY 195

NUMBER OF STATIONS =         25

NUMBER OF SUBREGIONS =          1

NUMBER OF METHOD PARAMETERS =         10

PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER         28

INPUT CARDS WILL BE PRINTED

OUTPUT GRID WILL BE PRINTED

UNIT TABLE WILL NOT BE PRINTED

STATION LOCATIONS WILL NOT BE PRINTED

SUBREGION GRID WILL NOT BE PRINTED

METHOD TABLE WILL NOT BE PRINTED

STATION VALUES WILL NOT BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       5.00

ENDING DATE OF FILE      76195 ENDING TIME OF FILE      24.00


REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
```

Exhibit VII-14. Sample Output from the TMPRTR Program

```
FILE NAME -- TEMPERATUR        TEMPERATURE FIELD FOR ST. LOUIS  DAY 195                                                  PAGE  1

TEMPERATURE VALUES (IN DEGREES KELVIN ATGROUND LEVEL)        VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00

GRID CELL        1          2          3          4          5          6          7          8          9         10         11         12

   22      292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000

   21      292.1000   292.1427   292.1843   292.2232   292.2577   292.2863   292.3070   292.3189   292.3246   292.3269   292.3273   292.3228

   20      292.1000   292.1868   292.2711   292.3501   292.4201   292.4774   292.5169   292.5343   292.5378   292.5351   292.5304   292.5189

   19      292.1000   292.2338   292.3639   292.4858   292.5944   292.6837   292.7434   292.7542   292.7425   292.7251   292.7118   292.6927

   18      292.1000   292.2853   292.4657   292.6351   292.7871   292.9168   293.0133   292.9875   292.9389   292.8914   292.8729   292.8534

   17      292.1000   292.3425   292.5791   292.8013   293.0000   293.1791   293.4000   293.2338   293.1201   293.0101   293.0106   293.0120

   16      292.1000   292.4059   292.7066   292.9893   293.2285   293.3913   293.4820   293.4164   293.2820   293.0000   293.1240   293.1685

   15      292.1000   292.4745   292.8510   293.2182   293.5277   293.6664   293.7068   293.6523   293.5701   293.4127   293.2920   293.2051

   14      292.1000   292.5407   293.0027   293.5015   293.9912   294.0301   294.0137   293.9000   293.9121   293.7621   293.4000   293.2309

   13      292.1000   292.5841   293.1153   293.7895   294.9000   294.4395   294.4049   294.3544   294.3960   294.3000   293.5706   293.2619

   12      292.1000   292.5780   293.0821   293.6364   294.2126   294.4150   294.8000   294.7025   295.0000   294.4038   293.3000   293.2116

   11      292.1000   292.5431   292.9955   293.4575   293.8931   294.2008   294.4509   294.6431   295.2000   295.0000   293.8000   293.2757

   10      292.1000   292.4966   292.8972   293.3018   293.6969   294.0384   294.1521   294.2098   294.2000   293.9881   293.2000   293.0827

    9      292.1000   292.4447   292.7934   293.1538   293.5514   294.1000   293.9037   293.8375   293.7469   293.5457   293.1952   292.9836

    8      292.1000   292.3887   292.6779   292.9673   293.2525   293.5040   293.5219   293.4857   293.4003   293.2491   293.0489   292.8701

    7      292.1000   292.3330   292.5633   292.7851   292.9863   293.1394   293.1922   293.1811   293.1178   293.0000   292.8803   292.7466

    6      292.1000   292.2812   292.4584   292.6247   292.7690   292.8751   292.9258   292.9278   292.8885   292.8151   292.7257   292.6252

    5      292.1000   292.2352   292.3666   292.4881   292.5915   292.6676   292.7088   292.7160   292.6931   292.6458   292.5825   292.5090

    4      292.1000   292.1951   292.2873   292.3720   292.4436   292.4968   292.5276   292.5357   292.5229   292.4929   292.4503   292.3992

    3      292.1000   292.1600   292.2183   292.2718   292.3170   292.3509   292.3714   292.3778   292.3713   292.3537   292.3275   292.2954

    2      292.1000   292.1288   292.1569   292.1827   292.2046   292.2211   292.2313   292.2349   292.2322   292.2241   292.2117   292.1963

    1      292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000   292.1000
```

Exhibit VII-14 (Continued)

```
FILE NAME -- TEMPERATUR        TEMPERATURE FIELD FOR ST. LOUIS  DAY 195                                                    PAGE  2

TEMPERATURE VALUES (IN DEGREES KELVIN ATGROUND LEVEL)        VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00

GRID CELL        13        14        15        16        17

     22     292.1000  292.1000  292.1000  292.1000  292.1000

     21     292.3098  292.2851  292.2458  292.1874  292.1000

     20     292.4899  292.4375  292.3584  292.2488  292.1000

     19     292.6503  292.5670  292.4482  292.2942  292.1000

     18     292.8037  292.6838  292.5207  292.3274  292.1000

     17     292.9857  292.7933  292.5759  292.3480  292.1000

     16     293.3000  292.8876  292.5972  292.3500  292.1000

     15     293.0997  292.8293  292.5434  292.3241  292.1000

     14     293.0325  292.7598  292.4000  292.2829  292.1000

     13     293.0157  292.7565  292.4927  292.2955  292.1000

     12     292.9955  292.7442  292.5077  292.2993  292.1000

     11     293.0000  292.7093  292.4890  292.2909  292.1000

     10     292.8676  292.6000  292.4457  292.2739  292.1000

      9     292.7846  292.5855  292.4193  292.2589  292.1000

      8     292.7009  292.5377  292.3870  292.2424  292.1000

      7     292.6112  292.4777  292.3489  292.2237  292.1000

      6     292.5197  292.4131  292.3076  292.2034  292.1000

      5     292.4297  292.3478  292.2651  292.1825  292.1000

      4     292.3428  292.2834  292.2227  292.1615  292.1000

      3     292.2593  292.2208  292.1811  292.1407  292.1000

      2     292.1787  292.1599  292.1402  292.1202  292.1000

      1     292.1000  292.1000  292.1000  292.1000  292.1000
```

Exhibit VII-14 (Concluded)

J. TERRAIN

The TERRAIN file contains time-invariant matrices of surface roughness and vegetation factors that are used by the Airshed Simulation Program to calculate vertical diffusivity and surface deposition. If the TERRAIN file is omitted from a simulation run, single values for surface roughness and vegetation factors will be used (see Section IX.B). The program TERAIN is used to create the TERRAIN file. TERAIN requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-19 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the TERAIN program.

1. Variables

The TERAIN program has two implicit output variables: ROUGHNESS and VEGFACTOR. The internal units for ROUGHNESS are meters (m); VEGFACTOR is the fraction of surface uptake capability compared to that of alfalfa. If the input values for ROUGHNESS are to be in any other units, that variable must be specified in the UNITS packet. VEGFACTOR is unitless; therefore, its units cannot be changed.

2. Methods

The methods that can be used to generate the TERRAIN file are:

> CONSTANT
> GRID VALUE
> STATINTERP
> POISSON
> E-WINTERP
> N-SINTERP
> USER.

These methods are discussed in detail in Section VI.A.6.

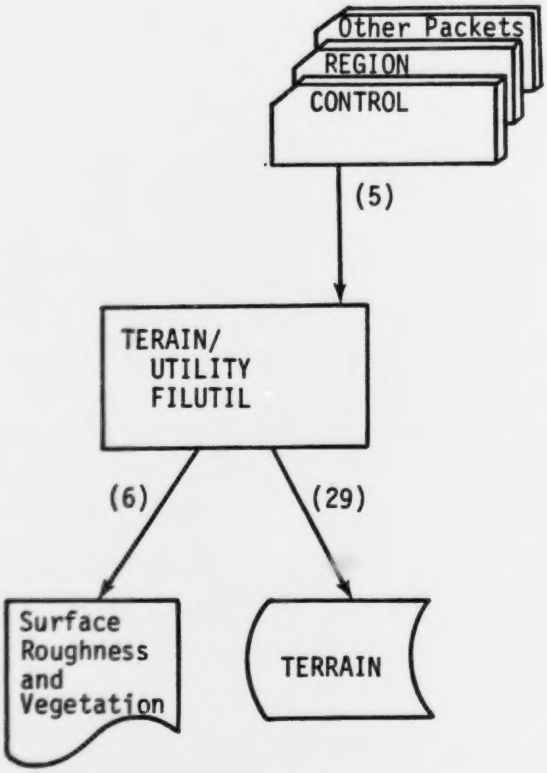

Other Packets
REGION
CONTROL
(5)
TERAIN/
UTILITY
FILUTIL
(6)
(29)
Surface
Roughness
and
Vegetation
TERRAIN

Figure VII-19. Information Flow Diagram for the TERRAIN File

3. Time Variation

The TERRAIN file contains values for surface characteristics that are considered to be invariant over time.

4. Packets

Figure VII-20 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the TERRAIN file:

> CONTROL
- The file name on Card 2 must be TERRAIN.
- The control variables to be specified on Cards 4 to 8 for TERRAIN are shown in Table VII-8.
- The number of species should be zero.
- If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.
- If data from measuring stations are to be used (methods STATINTERP or POISSON), the maximum number of such stations must be given.
- The number of subregions must be at least one.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) should be left blank.
- The file unit assignment card (No. 8) should be left blank.
- The beginning and ending dates and times can be any valid numbers. They are ignored by the Airshed Simulation Program.
- A set of output species names is not required; if they are present, their number must be the same as the entry in the first control parameter on Card 4, but they will be ignored by the program.

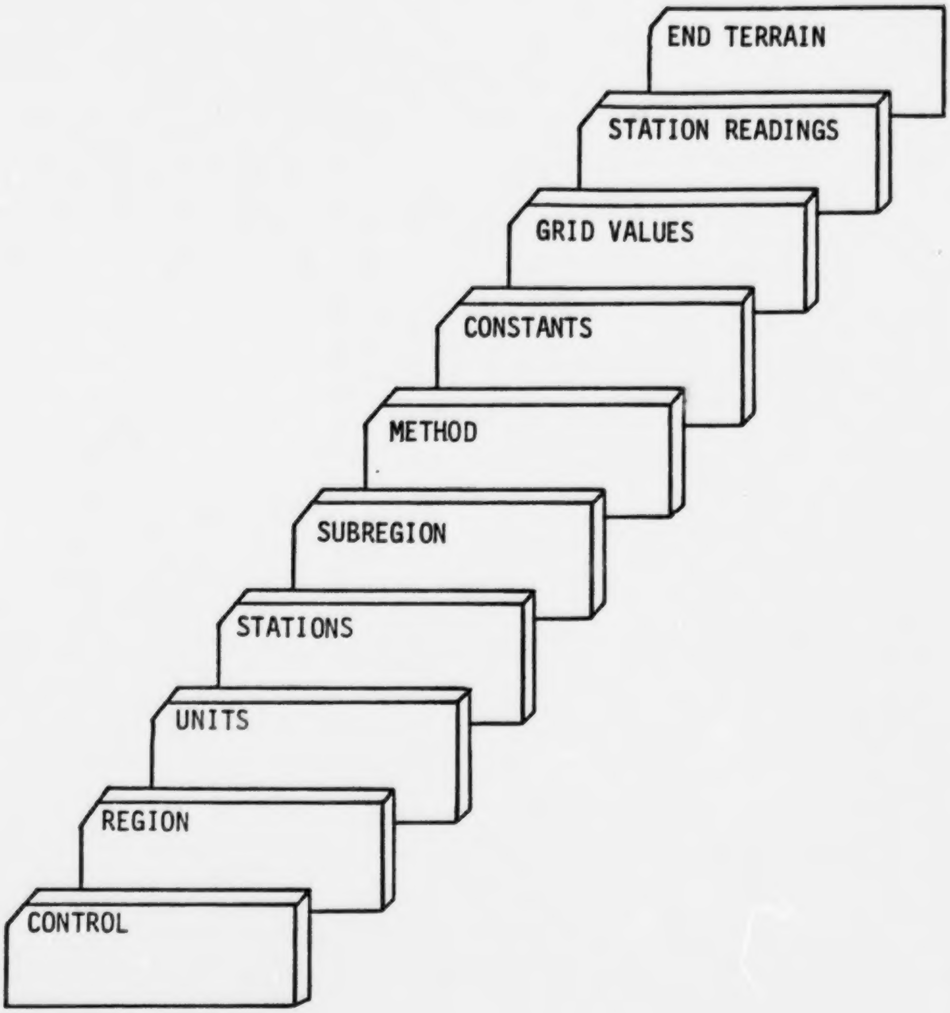

END TERRAIN
STATION READINGS
GRID VALUES
CONSTANTS
METHOD
SUBREGION
STATIONS
UNITS
REGION
CONTROL

Figure VII-20. Input Card Deck Structure for Preparing the TERRAIN File

Table VII-8. CONTROL Packet Entries for the TERRAIN File

Card Number	Entry
4	Number of species (=0)
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
8	Spare
	Spare
	Spare
	Spare
	Spare
	Spare

> REGION. This packet must follow the CONTROL packet. The vertical parameters will be ignored for the TERRAIN file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:
>
> - Any input variable will be input in other than internal units.
> - Any user-defined variables are specified.
> - COORD or HEIGHT unit conversions are to be used.
>
> The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> STATIONS. This packet is required if either method STATINTERP or POISSON is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.

> SUBREGION. A SUBREGION packet is required. The number of subregions must not exceed the maximum specified in the CONTROL packet.

> METHOD. A method must be provided for every variable--including user-defined variables--in every subregion. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, there must be one or more CONSTANTS packets.

> GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, there must be one or more GRID VALUES packets.

> STATION READINGS. If either the POISSON or STATINTERP method is assigned to any variable in the METHOD packet, there must be one or more STATION READINGS packets.

> END TERRAIN. This card must appear to indicate that no more packets are to be read.

5. Additional Input Files

No additional input files are required.

6. Examples

Exhibit VII-15 shows a sample input deck for TERRAIN file generation. The output from a TERAIN run using that input deck is shown in Exhibit VII-16.

```
CONTROL
TERRAIN
   SURFACE ROUGHNESS AND VEGETATIVE FACTORS
         0         0         0         1
        11         0         1
         0         0         0         1
         0
         0
     74001       000     78365      2400
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.       50.      200.
END
SUBREGION
A                  1         1        -1
END
METHOD
A         ALL       GRIDVALUE         0.      100.
END
GRIDVALUES
A         ROUGHNESS          1         1       .48
A         ROUGHNESS          2         1       .48
A         ROUGHNESS          3         1       .48
A         ROUGHNESS          4         1       .48
A         ROUGHNESS          5         1       .48
A         ROUGHNESS          6         1       .36
A         ROUGHNESS          7         1       .31
A         ROUGHNESS          8         1       .21
A         ROUGHNESS          9         1       .19
A         ROUGHNESS         10         1       .29
A         ROUGHNESS         11         1       .29
A         ROUGHNESS         12         1       .28
A         ROUGHNESS         13         1       .28
A         ROUGHNESS         14         1       .27
A         ROUGHNESS         15         1       .27
A         ROUGHNESS         16         1       .27
A         ROUGHNESS         17         1       .27
A         ROUGHNESS          1         2       .48
A         ROUGHNESS          2         2       .48
A         ROUGHNESS          3         2       .48
A         ROUGHNESS          4         2       .48
A         ROUGHNESS          5         2       .48
A         ROUGHNESS          6         2       .36
A         ROUGHNESS          7         2       .31
```

Exhibit VII-15.   Sample Input Deck from the TERAIN Program

```
A          ROUGHNESS        8        2       .21
A          ROUGHNESS        9        2       .19
A          ROUGHNESS       10        2       .29
A          ROUGHNESS       11        2       .29
A          ROUGHNESS       12        2       .28
A          ROUGHNESS       13        2       .28
A          ROUGHNESS       14        2       .27
A          VEGFACTOR        2       21      1.00
A          VEGFACTOR        3       21      1.00
A          VEGFACTOR        4       21      1.00
A          VEGFACTOR        5       21      1.00
A          VEGFACTOR        6       21      1.00
A          VEGFACTOR        7       21      1.00
A          VEGFACTOR        8       21      1.00
A          VEGFACTOR        9       21      1.00
A          VEGFACTOR       10       21      1.00
A          VEGFACTOR       11       21      1.00
A          VEGFACTOR       12       21      1.00
A          VEGFACTOR       13       21      1.00
A          VEGFACTOR       14       21      1.00
A          VEGFACTOR       15       21      1.00
A          VEGFACTOR       16       21      1.00
A          VEGFACTOR       17       21      1.00
A          VEGFACTOR        1       22      1.00
A          VEGFACTOR        2       22      1.00
A          VEGFACTOR        3       22      1.00
A          VEGFACTOR        4       22      1.00
A          VEGFACTOR        5       22      1.00
A          VEGFACTOR        6       22      1.00
A          VEGFACTOR        7       22      1.00
A          VEGFACTOR        8       22      1.00
A          VEGFACTOR        9       22      1.00
A          VEGFACTOR       10       22      1.00
A          VEGFACTOR       11       22      1.00
A          VEGFACTOR       12       22      1.00
A          VEGFACTOR       13       22      1.00
A          VEGFACTOR       14       22      1.00
A          VEGFACTOR       15       22      1.00
A          VEGFACTOR       16       22      1.00
A          VEGFACTOR       17       22      1.00
END
ENDTERRAIN
```

Exhibit VII-15 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE TERRAIN

   SURFACE ROUGHNESS AND VEGETATIVE FACTORS


REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00     200.00
END
KCRNT =    41  NSCLFT = 26960  IN SCRSET
KCRNT =    81  NSCLFT = 26920  IN SCRSET
KCRNT =    85  NSCLFT = 26916  IN SCRSET
KCRNT =    89  NSCLFT = 26912  IN SCRSET
KCRNT =    93  NSCLFT = 26908  IN SCRSET
KCRNT =   103  NSCLFT = 26898  IN SCRSET
KCRNT =   477  NSCLFT = 26524  IN SCRSET
KCRNT =   479  NSCLFT = 26522  IN SCRSET
KCRNT =   481  NSCLFT = 26520  IN SCRSET
KCRNT =   483  NSCLFT = 26518  IN SCRSET
KCRNT =   485  NSCLFT = 26516  IN SCRSET
KCRNT =   487  NSCLFT = 26514  IN SCRSET
KCRNT =   861  NSCLFT = 26626  IN SCRSET
KCRNT =  1235  NSCLFT = 26252  IN SCRSET
KCRNT =  1983  NSCLFT = 25504  IN SCRSET
SUBREGION
METHOD


                                       METHODS TABLE

 SUBREGION       VARIABLE        METHOD        MIN. VALUE     MAX. VALUE       PARAMETER       PAR. VALUE


 A               ROUGHNESS       GRIDVALUE          .0000       100.0000
 A               VEGFACTOR       GRIDVALUE          .0000       100.0000
 GRIDVALUES
 ENDTERRAIN
```

Exhibit VII-16. Sample Output from the TERAIN Program

```
FILE NAME -- TERRAIN          SURFACE ROUGHNESS AND VEGETATIVE FACTORS                                        PAGE  1
TERRAIN VALUES (IN METERS OR ALFALFA EQUIVALENTS) ROUGHNESS  VERT.  LEVEL 1 START DATE/TIME     0   .00 STOP DATE/TIME     0   .00
GRID CELL       1         2         3         4         5         6         7         8         9        10        11        12
   22         .2300     .2300     .2300     .2300     .2300     .2800     .2900     .2600     .2900     .2800     .2500     .2800
   21         .2300     .2300     .2300     .2300     .2300     .2800     .2900     .2600     .2900     .2800     .2500     .2800
   20         .2300     .2300     .2300     .2300     .2300     .2800     .2900     .2600     .2900     .2800     .2500     .2800
   19         .2200     .2200     .2200     .2200     .2200     .2700     .2800     .2500     .2700     .3400     .3200     .2600
   18         .2100     .2100     .2100     .2100     .2100     .2600     .2700     .2500     .2400     .1600     .1600     .5100
   17         .2200     .2200     .2200     .2200     .2200     .2600     .2700     .2500     .2400     .1500     .1500     .2700
   16         .2900     .2900     .2900     .2900     .2900     .3800     .5200     .4400     .3600     .2300     .1700     .1900
   15         .4400     .4400     .4400     .4400     .4400     .5900     .6700     .5700     .5100     .3400     .1800     .2000
   14         .6400     .6400     .6400     .6400     .6400     .7800     .7400     .6600     .6900     .2300     .3900     .4800
   13         .6700     .6700     .6700     .6700     .6700     .8000     .7400     .9400    1.5500     .4200     .6800     .2100
   12         .5900     .5900     .5900     .5900     .5900     .6300     .6600    2.0100    3.1700    1.7800     .3900     .3900
   11         .5800     .5800     .5800     .5800     .5800     .5800     .6700    1.2000    2.2000    1.2000    1.1200     .6700
   10         .8200     .8200     .8200     .8200     .8200     .8800     .8400    1.8400    2.2400     .5400     .3700     .4800
    9         .5400     .5400     .5400     .5400     .5400     .5300     .5200     .5600     .5500     .3800     .3300     .3400
    8         .4700     .4700     .4700     .4700     .4700     .5400     .5600     .4500     .2300     .4100     .3000     .3000
    7         .4700     .4700     .4700     .4700     .4700     .4900     .4800     .3700     .2300     .2800     .3400     .3400
    6         .4900     .4900     .4900     .4900     .4900     .3800     .3300     .2300     .2100     .3400     .2900     .3000
    5         .4800     .4800     .4800     .4800     .4800     .3600     .3100     .2100     .1900     .2900     .2800     .2800
    4         .4800     .4800     .4800     .4800     .4800     .3600     .3100     .2100     .1900     .2900     .2900     .2800
    3         .4800     .4800     .4800     .4800     .4800     .3600     .3100     .2100     .1900     .2900     .2900     .2800
    2         .4800     .4800     .4800     .4800     .4800     .3600     .3100     .2100     .1900     .2900     .2900     .2800
    1         .4800     .4800     .4800     .4800     .4800     .3600     .3100     .2100     .1900     .2900     .2900     .2800
```

Exhibit VII-16 (Continued)

```
FILE NAME -- TERRAIN          SURFACE ROUGHNESS AND VEGETATIVE FACTORS                                     PAGE  1
TERRAIN VALUES (IN METERS OR ALFALFA EQUIVALENTS) VEGFACTOR  VERT.  LEVEL 1 START DATE/TIME     0   .00 STOP DATE/TIME     0   .00
 GRID CELL        1         2         3         4         5         6         7         8         9        10        11        12
     22        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     21        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     20        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     19        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     18        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     17        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     16        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     15        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
     14        1.0000    1.0000    1.0000    1.0000    1.0000     .5000     .5000    1.0000    1.0000    1.0000    1.0000    1.0000
     13        1.0000    1.0000    1.0000    1.0000    1.0000     .5000     .5000     .5000     .5000    1.0000    1.0000    1.0000
     12        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000     .5000     .5000     .5000    1.0000    1.0000
     11        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000     .5000     .5000     .5000     .5000    1.0000
     10         .5000     .5000     .5000     .5000     .5000     .5000     .5000     .5000     .5000    1.0000    1.0000    1.0000
      9        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      8        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      7        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      6        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      5        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      4        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      3        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      2        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
      1        1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000    1.0000
```

Exhibit VII-16 (Concluded)

K. TOPCONC

The TOPCONC file contains time-varying matrices of pollutant concentrations at the top of the region. The program TPCONC is used to create the TOPCONC file. TPCONC requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-21 is an information flow diagram illustrating the job control to be used. The following sections discuss the input to the TPCONC program.

1. Variables

The output variables for the TOPCONC file are the species named in the CONTROL packet. Additional user-defined input variables (e.g. "reactive hydrocarbons") can be specified in the UNITS packet. THe internal units for the concentrations of all species except AEROSOLS are parts per million (ppm); for AEROSOLS, the units are micrograms per cubic meter ($\mu g/m^3$). The standard names for reactive species recognized by the Airshed Simulation Program are listed in Section IX.A. If any of these species does not appear on the TOPCONC file, the top concentrations will default to a value defined in the CHEMPARAM file. If any additional species appear on TOPCONC, they will be ignored.

2. Methods

The methods that can be used to generate the TOPCONC file are:

> CONSTANT
> GRID VALUE
> STATINTERP
> POISSON
> SPLIT/COMB
> ABSTOPCONC
> RELTOPCONC

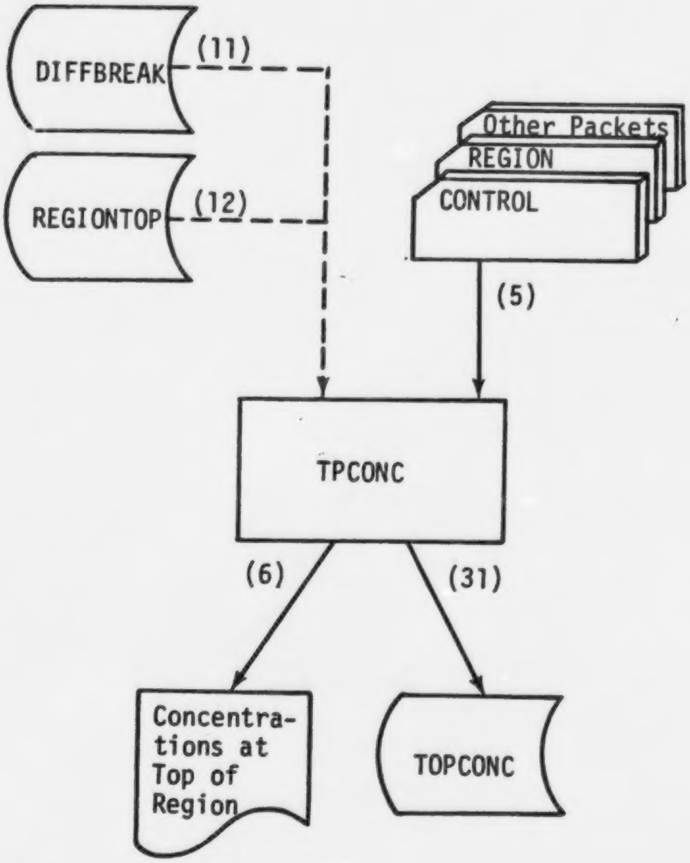

DIFFBREAK
(11)
REGIONTOP
(12)
Other Packets
REGION
CONTROL
(5)
TPCONC
(6)
(31)
Concentrations at Top of Region
TOPCONC

Figure VII-21. Information Flow Diagram for the TOPCONC File

- > E-WINTERP
- > N-SINTERP
- > USER.

These methods are discussed in detail in Section VI.A.6.

3. Time Variation

The time span of the TOPCONC file must include the entire time span of the simulation runs for which it is to be used. Concentrations at the top of the region are considered to be constant during each time interval.

4. Packets

Figure VII-22 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the TOPCONC file.

- > CONTROL
    - The file name on Card 2 must be TOPCONC.
    - The control variables to be specified on Cards 4 to 8 for TOPCONC are shown in Table VII-9.
    - The number of species must be greater than zero.
    - If there are input variables that do not appear as output variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.
    - If data from measuring stations are to be used (methods STATINTERP or POISSON), the maximum number of such stations must be given.
    - The number of subregions must be at least one.
    - The maximum number of parameters must be sufficient to include all specification of all parameters.

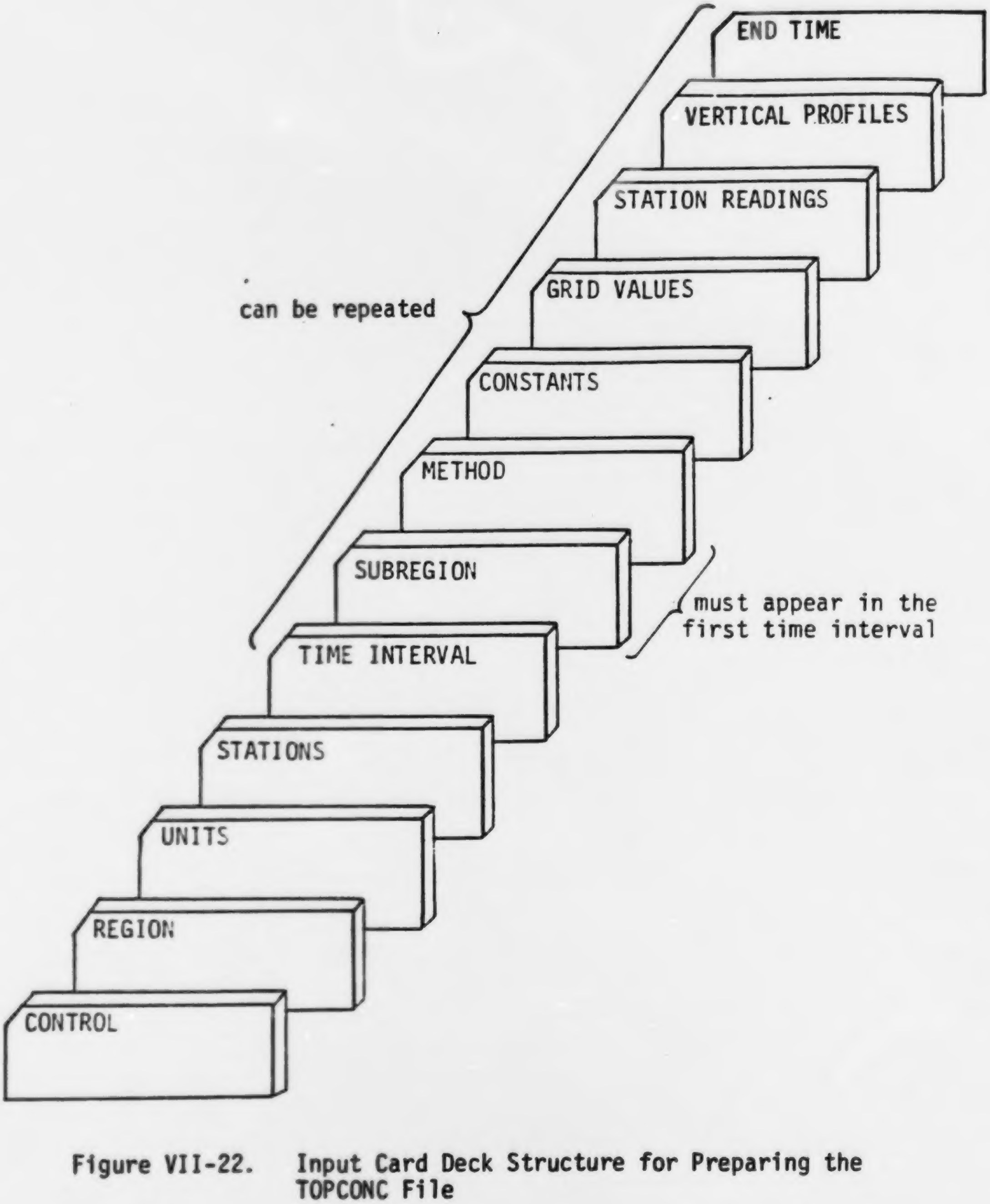

END TIME
VERTICAL PROFILES
STATION READINGS
GRID VALUES
CONSTANTS
METHOD
SUBREGION
TIME INTERVAL
STATIONS
UNITS
REGION
CONTROL
can be repeated
must appear in the first time interval

Figure VII-22. Input Card Deck Structure for Preparing the TOPCONC File

Table VII-9. CONTROL Packet Entries for the TOPCONC File

Card Number	Entry
4	Number of species
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print output grid
	Spare
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Spare
	Number of heights in profile
	Spare
	Print vertical profile tables
	Spare
	Spare
8	DIFFBREAK file number
	REGIONTOP file number
	Spare
	Spare
	Spare
	Spare

- The vertical controls card (No. 7) must contain the maximum number of profile heights if ABSTOPCONC or RELTOPCONC is used. Otherwise, this card should be blank.
- The file unit assignment card (No. 8) must provide an entry for REGIONTOP if the method ABSTOPCONC or RELTOPCONC is selected. It must also provide an entry for DIFFBREAK if RELTOPCONC is selected.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is required; their number must be the same as the entry in the first control parameter on Card 4.

> REGION. This packet must follow the CONTROL packet. The vertical parameters will be ignored for the TOPCONC file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:

- Any input variable will be input in other than internal units.
- Any user-defined variables are specified.
- COORD or HEIGHT unit conversions are to be used.

The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> STATIONS. This packet is required if the method STATINTERP or POISSON is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.

> TIME INTERVAL. One or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

- SUBREGION. The first time interval must contain a SUBREGION packet; the inclusion of this packet in other time intervals is optional. The number of subregions must not exceed the maximum specified in the CONTROL packet.
- METHOD. A method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that *each* parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.
- CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.
- GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, the first time interval must contain a GRID VALUES packet. More than one GRID VALUES packet can appear in any time interval.
- STATION READINGS. If either the POISSON or STATINTERP method is assigned to any species in the METHOD packet, the first time interval must contain a STATION READINGS packet. More than one STATION READINGS packet can appear in any time interval.
- VERTICAL PROFILES. If the method ABSTOPCONC or RELTOPCONC is assigned to any species in the METHOD packet, the first time interval must contain a VERTICAL PROFILES packet. There must be a vertical profile defined (or implied by means of ALL) for every variable in every subregion for which the profile method was specified. The number of height-value pairs in any single profile must not exceed the maximum specified in the CONTROL packet. More than one VERTICAL PROFILES packet can appear in any time interval.

5. Additional Input Files

If the method ABSTOPCONC or RELTOPCONC was selected, the REGIONTOP file must be input to TPCONC. In addition, if the method RELTOPCONC was selected, the DIFFBREAK file must also be input.

6. Examples

Exhibit VII-17 shows a sample input deck for TOPCONC file generation. The output from a TPCONC run using that input deck is shown in Exhibit VII-18.

```
CONTROL
TOPCONC
   POLLUTANT CONCENTRATIONS ABOVE THE MODELING REGION
        11         0         0         1         0
        31         1         1
         1         1         1         1         0
                   0                   0
NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
     76195       000     76195      2400
END
REGION
   725000.  4252000.        15
   -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2        0.       50.      200.
END
TIME INTERVAL
     76195       000     76195      2400
SUBREGION
A                  1         1        -1
END
METHOD
  A       NO        CONSTANT     .0001       .01
  A       NO2       CONSTANT     .0001       .01
  A       O3        CONSTANT      .001        .2
  A       ETH       CONSTANT     .0001       .01
  A       OLE       CONSTANT     .0001       .01
  A       PAR       CONSTANT      0.01        1.
  A       CARB      CONSTANT      .001       0.1
  A       ARO       CONSTANT     .0001       0.1
  A       BZA       CONSTANT   .000000     .0001
  A       PAN       CONSTANT   .000001     .0001
  A       CO        CONSTANT       .01        1.
END
```

Exhibit VII-17. Sample Input Deck for the TPCONC Program

```
CONSTANTS
  A        NO              .001
  A        NO2            .002
  A        O3              .078
  A        ETH           .00109
  A        OLE           .00220
  A        PAR           .03333
  A        CARB          .00405
  A        ARO           .00124
  A        BZA
  A        PAN           .00001
  A        CO               0.1
END
ENDTIME
```

Exhibit VII-17 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE TOPCONC

   POLLUTANT CONCENTRATIONS ABOVE THE MODELING REGION

NUMBER OF USER-DEFINED VARIABLES =          0

NUMBER OF STATIONS =          0

NUMBER OF SUBREGIONS =          1

NUMBER OF METHOD PARAMETERS =          0

NUMBER OF VERTICAL PROFILE HEIGHTS =          0

PROGRAM OUTPUT WILL BE PLACED ON FILE NUMBER        31

INPUT CARDS WILL BE PRINTED

OUTPUT GRID WILL BE PRINTED

UNIT TABLE WILL BE PRINTED

STATION LOCATIONS WILL BE PRINTED

SUBREGION GRID WILL BE PRINTED

METHOD TABLE WILL BE PRINTED

STATION VALUES WILL NOT BE PRINTED

VERTICAL PROFILE VALUES WILL NOT BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE        .00

ENDING DATE OF FILE      76195 ENDING TIME OF FILE      24.00

A TOTAL OF         11 SPECIES NAMES WERE READ, THE SPECIES NAMES ARE --

NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
```

Exhibit VII-18. Sample Output from the TPCONC Program

```
FILE NAME -- TOPCONC            POLLUTANT CONCENTRATIONS ABOVE THE MODELING REGION                                          PAGE  1
TOP CONCENTRATIONS ( IN PARTS PER MILLION) SPECIES NO         VERT.  LEVEL 1 START DATE/TIME 76195   0.00 STOP DATE/TIME 76195 24.00
 GRID CELL       1        2        3        4        5        6        7        8        9       10       11       12
    22        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    21        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    20        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    19        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    18        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    17        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    16        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    15        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    14        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    13        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    12        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    11        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
    10        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     9        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     8        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     7        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     6        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     5        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     4        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     3        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     2        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
     1        .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010    .0010
```

Exhibit VII-18 (Continued)

```
FILE NAME -- TOPCONC          POLLUTANT CONCENTRATIONS ABOVE THE MODELING REGION                              PAGE  2
TOP CONCENTRATIONS (IN PARTS PER MILLION) SPECIES NO      VERT.  LEVEL 1 START DATE/TIME 76195  0.00 STOP DATE/TIME 76195 24.00
GRID CELL       13        14        15        16        17
    22        .0010     .0010     .0010     .0010     .0010
    21        .0010     .0010     .0010     .0010     .0010
    20        .0010     .0010     .0010     .0010     .0010
    19        .0010     .0010     .0010     .0010     .0010
    18        .0010     .0010     .0010     .0010     .0010
    17        .0010     .0010     .0010     .0010     .0010
    16        .0010     .0010     .0010     .0010     .0010
    15        .0010     .0010     .0010     .0010     .0010
    14        .0010     .0010     .0010     .0010     .0010
    13        .0010     .0010     .0010     .0010     .0010
    12        .0010     .0010     .0010     .0010     .0010
    11        .0010     .0010     .0010     .0010     .0010
    10        .0010     .0010     .0010     .0010     .0010
     9        .0010     .0010     .0010     .0010     .0010
     8        .0010     .0010     .0010     .0010     .0010
     7        .0010     .0010     .0010     .0010     .0010
     6        .0010     .0010     .0010     .0010     .0010
     5        .0010     .0010     .0010     .0010     .0010
     4        .0010     .0010     .0010     .0010     .0010
     3        .0010     .0010     .0010     .0010     .0010
     2        .0010     .0010     .0010     .0010     .0010
     1        .0010     .0010     .0010     .0010     .0010
```

Exhibit VII-18 (Concluded)

L. WIND

The WIND file contains time-varying matrices of horizontal wind vector values in three dimensions and scalars representing overall maxima and average values at the boundaries. The program WNDSET is used to create the WIND file. WNDSET requires subroutines from the libraries UTILITY and FILUTIL. Figure VII-23 is an information flow diagram illustrating the job control to be used. In the following sections we discuss the input to the WNDSET program.

1. Variables

The WNDSET program has four implicit variables: SPEED, DIRECTION, WINDX, and WINDY. The first two represent a wind vector in polar form, and the latter two represent the vector in terms of its x- and y-components. A three-dimensional matrix is maintained for each variable. In general, the input to the program will be SPEED and DIRECTION, whereas the variables written to the WIND file are WINDX and WINDY. The WNDSET program calculates values for the undefined variables from those for variables to which values have been assigned.

2. Methods

The methods that can be used to generate the WIND file are:

- CONSTANT
- GRID VALUE
- STATINTERP
- POISSON
- DIVERGENCE
- VECTORIZE
- POLARIZE

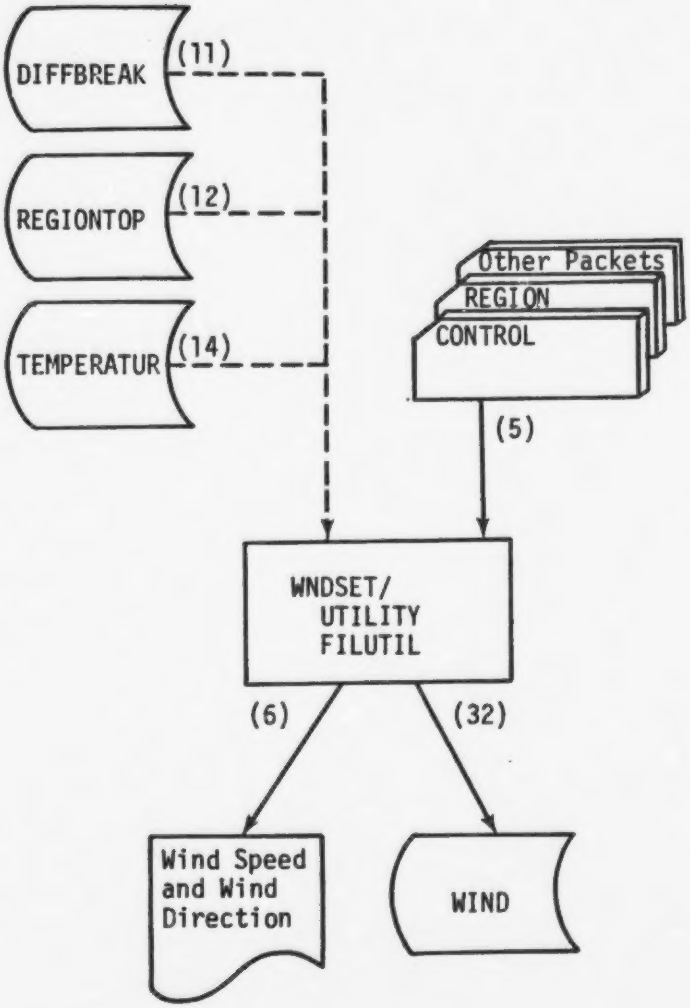

DIFFBREAK
(11)
REGIONTOP
(12)
TEMPERATUR
(14)
Other Packets
REGION
CONTROL
(5)
WNDSET/
UTILITY
FILUTIL
(6)
(32)
Wind Speed and Wind Direction
WIND

Figure VII-23. Information Flow Diagram for the WIND File

> E-WINTERP
> N-SINTERP
> USER.

These methods are discussed in detail in Section VI.A.6.

Since the WIND file varies in the vertical direction, a vertical method must also be specified for each output variable in each subregion. The vertical methods that can be used are:

> CONSTANT
> ABSPROFILE
> RELPROFILE
> DIVERGENCE
> VECTORIZE
> POLARIZE
> E-WINTERP
> N-SINTERP
> VERTUSER.

These vertical methods are discussed in detail in Section VI.A.6.

3. Time Variation

The time span of the WIND file must include the entire time span of the simulation runs for which it is to be used. Wind vectors and scalar values are considered to be constant during each time interval.

4. Packets

Figure VII-24 shows the input deck structure in terms of the packets to be used. Each of these packets is described in detail in Section VI.B. Following are special input packet considerations for the WIND file:

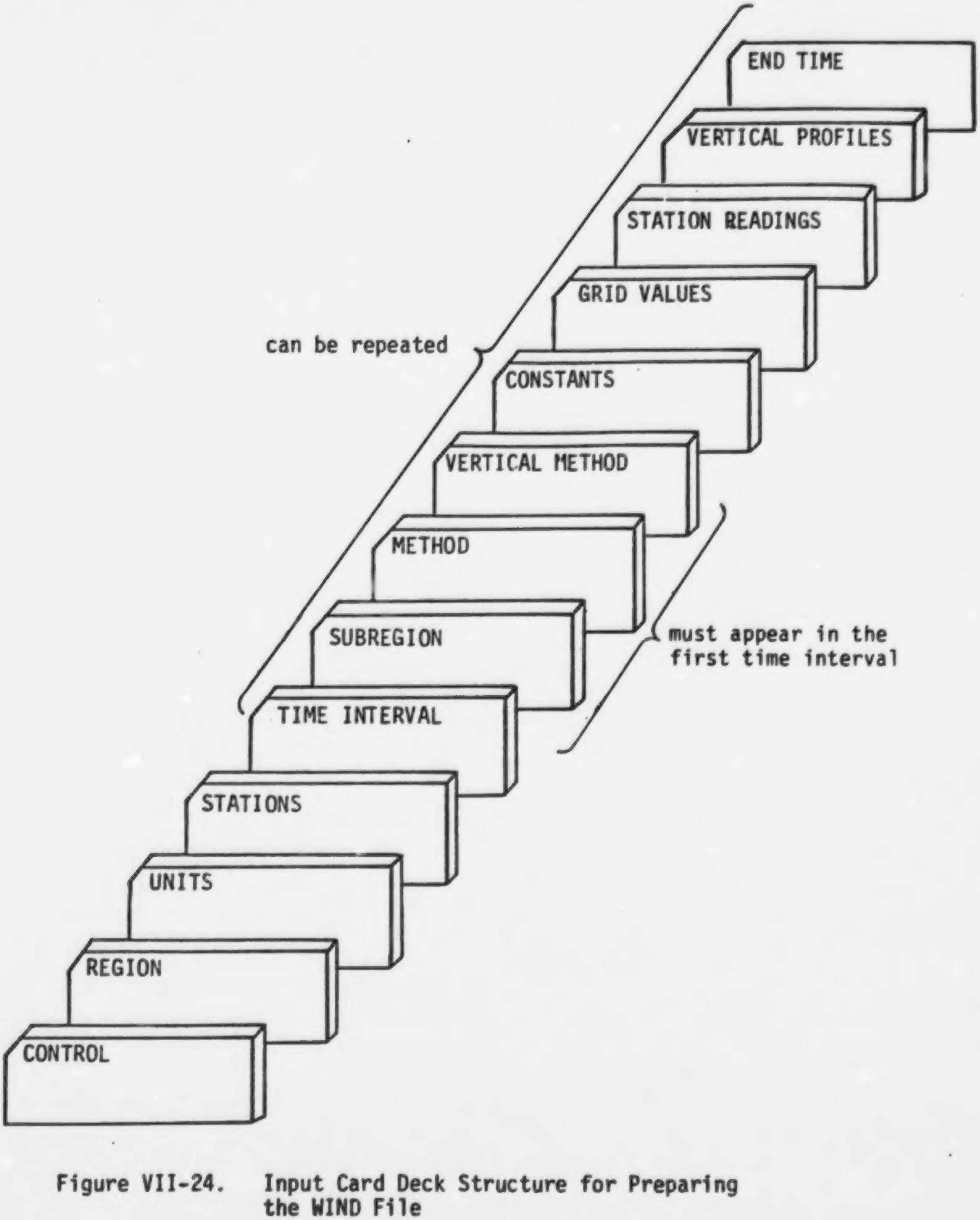

END TIME
VERTICAL PROFILES
STATION READINGS
GRID VALUES
can be repeated
CONSTANTS
VERTICAL METHOD
METHOD
SUBREGION
must appear in the first time interval
TIME INTERVAL
STATIONS
UNITS
REGION
CONTROL

Figure VII-24. Input Card Deck Structure for Preparing the WIND File

> CONTROL

- The file name on Card 2 must be WIND.
- The control variables to be specified on Cards 4 to 8 for WIND are shown in Table VII-10.
- The number of species should be zero.
- If there are input variables other than the four implicit variables, their number must appear as the number of user-defined variables. All such variables must also be named in the UNITS packet.
- If data from measuring stations are to be used (methods STATINTERP, POISSON, or DIVERGENCE), the maximum number of such stations must be given.
- The number of subregions must be at least one.
- The maximum number of parameters must be sufficient to include all specifications of all parameters.
- The vertical controls card (No. 7) must include maximum vertical parameter and profile entries as applicable.
- The file unit assignment card (No. 8) must provide entries for DIFFBREAK and REGIONTOP if any vertical method besides CONSTANT is selected. In addition, entries for TEMPERATUR must appear if DIVERGENCE is used.
- The beginning and ending dates and times should reflect the time variation considerations discussed in Section 3 above.
- A set of output species names is not required; if they are present, their number must be the same as the entry in the first control parameter on Card 4, but they will be ignored by the program.

> REGION. This packet must follow the CONTROL packet. The vertical parameters must be provided for the WIND file.

> UNITS. This packet, if present, must follow the REGION packet. The UNITS packet must be provided if:

- Any input variable will be input in other than internal units.

Table VII-10. CONTROL Packet Entries for the WIND File

Card Number	Entry
4	Number of species (=0)
	Number of user-defined variables
	Number of stations
	Number of subregions
	Number of parameters
	Spare
5	Output file number
	Print input cards
	Print grids for x- and y-components
	Print grids for speed and direction
	Spare
	Spare
6	Print units table
	Print station locations table
	Print regional grid
	Print methods table
	Print station values table
	Spare
7	Number of vertical parameters
	Number of heights in profile
	Print vertical methods table
	Print vertical profile tables
	Spare
	Spare
8	DIFFBREAK file number
	REGIONTOP file number
	Spare
	TEMPERATUR file number
	Spare
	Spare

- Any user-defined variables are specified.
- COORD or HEIGHT unit conversions are to be used.

The number of user-defined variables must not exceed the maximum specified in the CONTROL packet.

> STATIONS. This packet is required if any of the methods STATINTERP, POISSON, or DIVERGENCE is specified. The number of stations listed must not exceed the maximum specified in the CONTROL packet.

> TIME INTERVAL. One or more TIME INTERVAL packets must be present. The first time interval must begin at or before the beginning of the time span specified on Card 10 of the CONTROL packet. All time intervals must be contiguous and of nonzero length. Each TIME INTERVAL packet contains one or more of the following packets and ends with an ENDTIME card. Following the first time interval, only those data that are to be changed need be specified.

> SUBREGION. The first time interval must contain a SUBREGION packet; the inclusion of this packet in other time intervals is optional. The number of subregions must not exceed the maximum specified in the CONTROL packet.

> METHOD. A method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each parameter entry contributes to the overall parameter count; the total number of parameters must not exceed the maximum specified in the CONTROL packet.

> VERTICAL METHOD. A vertical method must be provided for every variable--including user-defined variables--in every subregion in the first time interval. Vertical methods can be changed in subsequent TIME INTERVAL packets if desired. Note that each vertical parameter entry contributes to the overall vertical parameter count; the total must not exceed the maximum specified in the CONTROL packet.

- CONSTANTS. If the method CONSTANT is assigned to any variable in the METHOD packet, the first time interval must contain a CONSTANTS packet. More than one CONSTANTS packet can appear in any time interval.
- GRID VALUES. If the method GRID VALUE is assigned to any variable in the METHOD packet, the first time interval must contain a GRID VALUES packet. More than one GRID VALUES packet can appear in any time interval.
- STATION READINGS. If either the POISSON, DIVERGENCE, or STATINTERP method is assigned to any variable in the METHOD packet, the first time interval must contain a STATION READINGS packet. More than one STATION READINGS packet can appear in any time interval.
- VERTICAL PROFILES. If any of the profile methods are assigned to any variable in the VERTICAL METHOD packet, the first time interval must contain a VERTICAL PROFILES packet. There must be a vertical profile defined (or implied by means of ALL) for every variable in every subregion for which a profile method was specified. The number of height-value pairs in any single profile must not exceed the maximum specified in the CONTROL packet. More than one VERTICAL PROFILES packet can appear in any time interval.

Typically, the wind values input will be in terms of SPEED and DIRECTION at measuring stations, whereas the variables output to the file are WINDX and WINDY. In this case, the methods and vertical methods should be specified as follows:

- For SPEED and DIRECTION, use the method and vertical method POLARIZE if speed and direction grids are to be printed, or CONSTANT if they are not to be printed. If CONSTANT is chosen, supply a dummy CONSTANTS packet to give an arbitrary initial value to the SPEED and DIRECTION grids.
- For WINDX and WINDY, specify one of the methods using station readings--STATINTERP, POISSON, or DIVERGENCE--and the vertical method desired for computation.

In each time interval, missing values of WINDX and WINDY for station readings and vertical profiles will be calculated from SPEED and DIRECTION, and vice versa. To ensure that old values are replaced with the appropriate new values, the variables WINDX and WINDY must be cleared to -9. before reading in the data for a new time invertal. For station readings, the following can be done:

```
STATION READINGS                       STATION READINGS
ALL          WINDX          -9.        ALL      ALL     -9.
                                  or
ALL          WINDY          -9.
END
```

A shorthand method for clearing an entire vertical profile to -9. has also been provided--simply specify -9 as the number of profile heights, as shown in the following example:

```
VERTICAL PROFILES
A_________ALL____________4200.__________5000.________-9
END
```

5. Additional Input Files

If any vertical method besides CONSTANT was selected, the DIFFBREAK and REGIONTOP files must be input to WNDSET. In addition, if DIVERGENCE was selected the TEMPERATUR file must also be input.

6. Examples

Exhibit VII-19 shows a sample input deck for WIND file generation. The output from a WNDSET run using that input deck is shown in Exhibit VII-20.

```
CONTROL
WIND
   WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED
         0         0        25         1        10
        32         0         1         0
         1         0         0         0         1
        10        20         0         0
        11        12                  14
     76195       500     76195      2400
END
REGION
   725000.  4252000.        15
  -19000.   -16000.
     4000.     4000.
        17        22         4
         2         2       0.0       50.      200.
END
```

Exhibit VII-19. Sample Input Deck for the WINDSET Program

```
UNITS
WINDX     M/SEC       3600.                   1.
WINDY     M/SEC       3600.                   1.
SPEED     M/SEC       3600.                   1.
END
STATIONS
        101    19183.    27862.       30.
        102    17518.    34045.       30.
        103    22588.    30467.       30.
        104    22312.    25304.       30.
        105    18706.    24453.       30.
        106    13660.    25566.       30.
        107    15179.    30610.       30.
        108    23407.    39102.       10.
        109    30802.    27886.       30.
        110    22209.    20826.       10.
        111    13812.    20479.       30.
        112     8938.    28913.       30.
        113    12738.    37820.       30.
        114    19320.    45456.       10.
        115    32111.    45799.       10.
        116    37777.    38083.       10.
        117    35560.    20818.       10.
        118    18065.    11256.       10.
        119     4759.    18547.       30.
        120    -1921.    33909.       30.
        121     7414.    50376.       10.
        122    16631.    77223.       30.
        123    52320.    34378.       30.
        124    24275.   -15463.       30.
        125   -27555.    30240.       30.
END
TIME INTERVAL
      76195        500     76195       600
SUBREGION
A                    1         1        -1
END
METHOD
A          WINDX     DIVERGENCE      -20.        20.        3
 RMAXIT        1000.
 TLRNCE       10000.
 ROMEGA          1.4
A          WINDY     DIVERGENCE      -20.        20.        3
 RMAXIT        1000.
 TLRNCE       10000.
 ROMEGA          1.4
A          SPEED     CONSTANT          0.        20.
A          DIRECTION CONSTANT         -7.         7.
END
```

Exhibit VII-19 (Continued)

```
VERTICAL METHOD
A          WINDY     DIVERGENCE      -20.   -    20.
A          WINDX     DIVERGENCE      -20.        20.
A          SPEED     CONSTANT          0.        20.
A          DIRECTION CONSTANT         -7.         7.
END
CONSTANTS
A          SPEED            3.0
A          DIRECTION        3.14
END                                                             WINDS FOR  500
STATION READINGS
 ALL       ALL             -9.0
 101       SPEED            3.51
 101       DIRECTION        1.83
 102       SPEED            3.26
 102       DIRECTION        2.21
 103       SPEED            2.18
 103       DIRECTION        1.88
 104       SPEED            3.17
 104       DIRECTION        1.96
 105       SPEED            3.24
 105       DIRECTION        1.72
 106       SPEED            3.75
 106       DIRECTION        1.77
 107       SPEED            2.96
 107       DIRECTION        1.93
 108       SPEED            2.06
 108       DIRECTION        1.98
 109       SPEED            2.94
 109       DIRECTION        1.75
 110       SPEED            1.86
 110       DIRECTION        1.62
 111       SPEED            2.38
 111       DIRECTION        1.81
 112       SPEED            2.83
 112       DIRECTION        1.82
 113       SPEED            3.83
 113       DIRECTION        2.10
 114       SPEED            1.77
 114       DIRECTION        1.92
 115       SPEED            2.16
 115       DIRECTION        1.86
 116       SPEED            2.70
 116       DIRECTION        1.80
 117       SPEED            2.67
 117       DIRECTION        1.97
```

Exhibit VII-19 (Continued)

```
118     SPEED          -9.00
118     DIRECTION      -9.00
119     SPEED           3.24
119     DIRECTION       1.84
120     SPEED           3.21
120     DIRECTION       1.98
121     SPEED           2.68
121     DIRECTION       1.84
122     SPEED           2.51
122     DIRECTION       2.37
123     SPEED           2.26
123     DIRECTION       2.04
124     SPEED          -9.00
124     DIRECTION      -9.00
125     SPEED           3.12
125     DIRECTION       1.76
END
VERTICAL PROFILE
A          ALL          42948.0  79053.0      2        STA
      -9.0      -9.0
      -9.0      -9.0
A          SPEED        42948.0  79053.0     20        STA 141
        .0       2.7
      34.5       4.9
     116.1       6.8
     197.0       7.5
     276.7       6.0
     355.4       4.7
     433.2       5.1
     510.0       5.5
     586.0       6.9
     660.9       9.2
     734.2       9.2
     807.2      11.6
     880.2      10.5
     953.2      10.5
    1026.2      10.5
    1099.2       9.8
    1172.2       9.3
    1245.6       8.9
    1319.0       8.7
    1392.0       8.2
A          DIRECTION    42948.0  79053.0     20        STA 141
        .0       1.5
      34.5       1.7
     116.1       1.9
     197.0       2.0
     276.7       2.0
     355.4       2.2
     433.2       4.7
     510.0       5.4
     586.0       5.5
     660.9       5.6
```

Exhibit VII-19 (Continued)

```
     734.2       5.6
     807.2       5.6
     880.2       5.6
     953.2       5.7
    1026.2       5.7
    1099.2       5.7
    1172.2       5.7
    1245.6       5.7
    1319.0       5.6
    1392.0       5.6
END
ENDTIME
TIME INTERVAL
     76195       600     76195       700
STATION READINGS                                         WINDS FOR  600
 ALL       ALL          -9.0
 101       SPEED         3.29
 101       DIRECTION     2.07
 102       SPEED         3.17
 102       DIRECTION     2.15
 103       SPEED         2.56
 103       DIRECTION     2.16
 104       SPEED         2.54
 104       DIRECTION     2.28
 105       SPEED         2.69
 105       DIRECTION     2.34
 106       SPEED         2.90
 106       DIRECTION     2.16
 107       SPEED         2.96
 107       DIRECTION     2.13
 108       SPEED         2.64
 108       DIRECTION     2.15
 109       SPEED         2.87
 109       DIRECTION     2.04
 110       SPEED         2.05
 110       DIRECTION     2.25
 111       SPEED         2.45
 111       DIRECTION     2.20
 112       SPEED         3.16
 112       DIRECTION     2.01
 113       SPEED         3.92
 113       DIRECTION     2.13
 114       SPEED         1.95
 114       DIRECTION     2.05
 115       SPEED         2.50
 115       DIRECTION     1.92
 116       SPEED         2.97
 116       DIRECTION     1.89
 117       SPEED         3.31
 117       DIRECTION     2.16
 118       SPEED         2.99
 118       DIRECTION     2.10
 119       SPEED         2.70
 119       DIRECTION     2.18
 120       SPEED         3.20
 120       DIRECTION     2.31
 121       SPEED         3.08
```

Exhibit VII-19 (Concluded)

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE WIND

   WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED


REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
KCRNT =    61  NSCLFT = 11840  IN SCRSET
KCRNT =   121  NSCLFT = 11780  IN SCRSET
KCRNT =   127  NSCLFT = 11774  IN SCRSET
KCRNT =   133  NSCLFT = 11768  IN SCRSET
KCRNT =   139  NSCLFT = 11762  IN SCRSET
KCRNT =   389  NSCLFT = 11512  IN SCRSET
KCRNT =   489  NSCLFT = 11412  IN SCRSET
KCRNT =   514  NSCLFT = 11387  IN SCRSET
KCRNT =   539  NSCLFT = 11362  IN SCPSET
KCRNT =   564  NSCLFT = 11337  IN SCRSET
KCRNT =   574  NSCLFT = 11327  IN SCRSET
KCRNT =   948  NSCLFT = 10953  IN SCRSET
KCRNT =   952  NSCLFT = 10949  IN SCRSET
KCRNT =   956  NSCLFT = 10945  IN SCRSET
KCRNT =   960  NSCLFT = 10941  IN SCRSET
KCRNT =   964  NSCLFT = 10937  IN SCRSET
KCRNT =   968  NSCLFT = 10933  IN SCRSET
KCRNT =  1068  NSCLFT = 10833  IN SCRSET
KCRNT =  1078  NSCLFT = 10823  IN SCRSET
KCRNT =  1082  NSCLFT = 10819  IN SCRSET
KCRNT =  1086  NSCLFT = 10815  IN SCRSET
KCRNT =  1090  NSCLFT = 10811  IN SCRSET
KCRNT =  1094  NSCLFT = 10807  IN SCRSET
KCRNT =  1098  NSCLFT = 10803  IN SCRSET
KCRNT =  1198  NSCLFT = 10703  IN SCRSET
KCRNT =  1208  NSCLFT = 10693  IN SCRSET
KCRNT =  1212  NSCLFT = 10689  IN SCRSET
KCRNT =  1216  NSCLFT = 10685  IN SCRSET
KCRNT =  1296  NSCLFT = 10605  IN SCRSET
KCRNT =  1376  NSCLFT = 10525  IN SCRSET
KCRNT =  1750  NSCLFT = 10151  IN SCRSET
KCRNT =  2124  NSCLFT =  9777  IN SCRSET
KCRNT =  2498  NSCLFT =  9403  IN SCRSET
KCRNT =  2872  NSCLFT =  9029  IN SCRSET
KCRNT =  3246  NSCLFT =  8655  IN SCRSET
KCRNT =  9230  NSCLFT =  2671  IN SCRSET
KCRNT =  9604  NSCLFT =  2297  IN SCRSET
UNITS
STATIONS
```

Exhibit VII-20. Sample Output from the WINDSET Program

```
                              STATION IDENTIFICATION TABLE
STATION NAME      X-LOCATION(GRID SQ)  Y-LOCATION (GRID SQ)  STATION HEIGHT(METERS)

     101                 9.55                10.97                30.00
     102                 9.13                12.51                30.00
     103                10.40                11.62                30.00
     104                10.33                10.33                30.00
     105                 9.43                10.11                30.00
     106                 8.16                10.39                30.00
     107                 8.54                11.65                30.00
     108                10.60                13.78                10.00
     109                12.45                10.97                30.00
     110                10.30                 9.21                10.00
     111                 8.20                 9.12                30.00
     112                 6.98                11.23                30.00
     113                 7.93                13.45                30.00
     114                 9.58                15.36                10.00
     115                12.78                15.45                10.00
     116                14.19                13.52                10.00
     117                13.64                 9.20                10.00
     118                 9.27                 6.81                10.00
     119                 5.94                 8.64                30.00
     120                 4.27                12.48                30.00
     121                 6.60                16.59                10.00
     122                 8.91                23.31                30.00
     123                17.83                12.59                30.00
     124                10.82                  .13                30.00
     125                -2.14                11.56                30.00
TIME INTERVAL
     76195       500      76195       600
```

Exhibit VII-20 (Continued)

```
SUBREGION
METHOD
VERTICAL METHOD
                                                METHODS TABLE

SUBREGION      VARIABLE       METHOD        MIN. VALUE      MAX. VALUE      PARAMETER      PAR. VALUE

A              WINDX          DIVERGENCE    -72000.0000     72000.0000
A              WINDY          DIVERGENCE    -72000.0000     72000.0000
A              SPEED          CONSTANT            .0000     72000.0000
A              DIRECTION      CONSTANT          -7.0000         7.0000
CONSTANTS
STATION READINGS                                            WINDS FOR  500
VERTICAL PROFILE
ENDTIME
KCRNT =     21  NSCLFT =  2277  IN SCRSET
KCRNT =     41  NSCLFT =  2257  IN SCRSET
KCRNT =     45  NSCLFT =  2253  IN SCRSET
KCRNT =     49  NSCLFT =  2249  IN SCRSET
KCRNT =     69  NSCLFT =  2229  IN SCRSET
KCRNT =     89  NSCLFT =  2209  IN SCRSET
KCRNT =     93  NSCLFT =  2205  IN SCRSET
KCRNT =    467  NSCLFT =  1831  IN SCRSET
KCRNT =    841  NSCLFT =  1457  IN SCRSET


WIND SCALAR VALUES BETWEEN DATE 76195 / TIME  5.00 AND DATE 76195 / TIME  6.00

AVERAGE STATION REFERENCE HEIGHT      23.60 METERS

MAXIMUM SPEED IN X-DIRECTION   22453.18 METERS/HOUR

MAXIMUM SPEED IN Y-DIRECTION    9602.99 METERS/HOUR

AVERAGE SPEED AT WEST BORDER   14801.04 METERS/HOUR

AVERAGE SPEED AT EAST BORDER   14801.11 METERS/HOUR

AVERAGE SPEED AT SOUTH BORDER   14799.13 METERS/HOUR

AVERAGE SPEED AT NORTH BORDER   14798.96 METERS/HOUR
```

Exhibit VII-20 (Continued)

```
FILE NAME -- WIND             WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED                                    PAGE  1
WIND VELOCITIES   (IN METERS PER HOUR)  COMPONENT WINDX       VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL         1         2         3         4         5         6         7         8         9        10        11        12
     22     -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24
     21     -9608.41  -9597.95  -9579.41  -9568.13  -9560.89  -9556.42  -9554.05  -9553.15  -9553.21  -9553.97  -9555.34  -9557.28
     20     -9629.52  -9617.58  -9590.74  -9570.93  -9556.77  -9547.54  -9542.64  -9540.86  -9541.03  -9542.76  -9545.91  -9550.42
     19     -9639.70  -9629.26  -9598.60  -9572.82  -9552.85  -9539.38  -9532.62  -9530.53  -9530.89  -9533.54  -9538.42  -9545.61
     18     -9643.83  -9635.78  -9603.36  -9573.39  -9548.70  -9531.51  -9524.08  -9522.62  -9522.87  -9526.22  -9532.48  -9540.82
     17     -9644.58  -9639.11  -9606.02  -9573.32  -9545.04  -9524.29  -9517.11  -9516.83  -9515.88  -9520.07  -9528.19  -9537.93
     16     -9643.51  -9640.49  -9607.57  -9573.79  -9544.33  -9522.76  -9512.11  -9508.57  -9507.45  -9513.54  -9524.24  -9535.49
     15     -9641.41  -9640.50  -9608.27  -9574.50  -9545.05  -9523.00  -9509.68  -9503.90  -9502.55  -9506.55  -9516.48  -9530.33
     14     -9638.67  -9639.30  -9608.03  -9574.90  -9546.36  -9524.56  -9509.46  -9502.23  -9499.21  -9499.19  -9507.85  -9524.57
     13     -9635.44  -9636.88  -9606.73  -9574.58  -9547.76  -9527.51  -9512.23  -9502.66  -9495.58  -9491.19  -9498.89  -9519.23
     12     -9631.80  -9633.17  -9604.48  -9573.99  -9548.09  -9528.70  -9514.25  -9503.75  -9491.93  -9483.51  -9492.50  -9516.89
     11     -9627.67  -9627.86  -9600.59  -9571.54  -9546.27  -9527.42  -9514.08  -9504.30  -9493.14  -9483.70  -9490.80  -9516.09
     10     -9623.07  -9620.88  -9595.05  -9567.46  -9542.58  -9524.25  -9511.06  -9499.94  -9490.60  -9486.79  -9496.40  -9521.06
      9     -9618.20  -9612.45  -9588.23  -9563.00  -9538.46  -9521.13  -9509.01  -9498.25  -9491.60  -9492.15  -9503.50  -9525.90
      8     -9613.28  -9603.53  -9579.32  -9559.94  -9536.94  -9519.30  -9506.79  -9497.73  -9493.74  -9497.33  -9509.89  -9531.00
      7     -9608.43  -9600.24  -9578.86  -9557.41  -9536.29  -9519.35  -9507.22  -9499.57  -9497.39  -9502.89  -9516.07  -9535.96
      6     -9603.65  -9596.32  -9575.93  -9555.66  -9536.86  -9521.61  -9510.75  -9504.55  -9503.75  -9509.49  -9521.85  -9540.34
      5     -9598.84  -9591.76  -9572.87  -9554.95  -9539.02  -9526.22  -9517.22  -9512.42  -9512.33  -9517.57  -9528.28  -9544.21
      4     -9593.75  -9586.84  -9570.19  -9555.47  -9543.00  -9533.22  -9526.46  -9523.02  -9523.23  -9527.42  -9535.76  -9548.15
      3     -9587.81  -9581.43  -9568.03  -9557.36  -9548.92  -9542.55  -9538.25  -9536.14  -9536.39  -9539.18  -9544.63  -9552.80
      2     -9579.70  -9574.95  -9566.50  -9560.83  -9556.77  -9553.88  -9552.01  -9551.13  -9551.29  -9552.56  -9555.02  -9558.76
      1     -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24  -9566.24
```

Exhibit VII-20 (Continued)

```
FILE NAME -- WIND             WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED                               PAGE  2
WIND VELOCITIES   (IN METERS PER HOUR)  COMPONENT WINDX      VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL       13        14        15        16        17
    22     -9566.24  -9566.24  -9566.24  -9566.24  -9566.24
    21     -9559.75  -9562.87  -9567.58  -9574.91  -9578.55
    20     -9556.05  -9561.82  -9570.62  -9582.49  -9586.79
    19     -9556.27  -9562.33  -9574.61  -9589.70  -9593.28
    18     -9551.24  -9563.53  -9579.54  -9597.14  -9598.94
    17     -9549.96  -9565.47  -9584.86  -9604.72  -9604.12
    16     -9549.26  -9567.40  -9590.16  -9612.26  -9609.00
    15     -9547.77  -9569.70  -9595.53  -9619.70  -9613.69
    14     -9545.83  -9571.59  -9600.60  -9626.83  -9618.20
    13     -9544.25  -9573.41  -9605.34  -9633.48  -9622.57
    12     -9544.28  -9575.70  -9609.89  -9639.59  -9626.94
    11     -9545.81  -9578.68  -9614.32  -9645.04  -9631.46
    10     -9550.51  -9583.39  -9618.79  -9649.68  -9636.27
     9     -9554.72  -9587.83  -9622.96  -9653.00  -9641.28
     8     -9558.72  -9590.80  -9624.42  -9653.57  -9645.85
     7     -9561.93  -9590.70  -9621.48  -9650.46  -9649.26
     6     -9563.83  -9582.33  -9613.42  -9644.51  -9650.73
     5     -9564.38  -9585.54  -9610.81  -9640.02  -9649.32
     4     -9564.13  -9582.82  -9605.28  -9632.82  -9643.69
     3     -9563.68  -9577.48  -9595.45  -9619.94  -9631.59
     2     -9563.98  -9571.18  -9581.71  -9598.90  -9608.83
     1     -9566.24  -9566.24  -9566.24  -9566.24  -9566.24
```

Exhibit VII-20 (Continued)

```
FILE NAME -- WIND            WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED
                                                                                                    PAGE  1
WIND VELOCITIES   (IN METERS PER HOUR)  COMPONENT WINDY      VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL          1          2          3          4          5          6          7          8          9         10         11         12
    22        3119.40    3161.58    3180.31    3185.97    3183.71    3176.66    3167.01    3156.30    3145.39    3134.84    3125.04    3116.40
    21        3119.40    3152.35    3170.68    3178.39    3178.33    3172.83    3163.96    3153.45    3142.37    3131.53    3121.70    3113.60
    20        3119.40    3136.33    3149.15    3155.83    3156.53    3152.41    3145.25    3137.09    3128.60    3120.44    3113.50    3108.58
    19        3119.40    3127.43    3134.67    3138.66    3138.49    3134.46    3128.06    3122.24    3116.30    3110.66    3106.48    3104.55
    18        3119.40    3122.24    3125.32    3126.90    3125.90    3121.98    3115.80    3112.40    3108.25    3103.97    3101.59    3100.84
    17        3119.40    3119.21    3119.65    3119.87    3119.29    3117.67    3114.93    3111.19    3106.77    3102.02    3100.30    3099.76
    16        3119.40    3117.45    3116.27    3115.86    3116.23    3117.51    3118.89    3115.10    3111.41    3107.45    3103.42    3100.82
    15        3119.40    3116.33    3114.04    3113.03    3113.59    3115.98    3118.37    3117.57    3116.92    3114.48    3107.52    3102.53
    14        3119.40    3115.54    3112.34    3110.55    3110.55    3113.38    3116.92    3119.12    3119.69    3116.66    3108.76    3103.24
    13        3119.40    3114.90    3110.92    3108.45    3107.91    3109.45    3112.72    3116.09    3117.01    3112.68    3105.14    3101.36
    12        3119.40    3114.30    3109.46    3105.90    3103.96    3102.56    3102.94    3104.28    3105.10    3103.27    3099.26    3097.51
    11        3119.40    3113.73    3107.95    3102.78    3098.29    3094.01    3091.04    3088.53    3085.43    3086.46    3088.70    3091.05
    10        3119.40    3113.45    3107.16    3100.83    3094.62    3088.26    3083.76    3078.84    3073.46    3074.10    3080.12    3085.96
     9        3119.40    3113.63    3107.79    3101.13    3095.10    3089.57    3084.33    3079.58    3076.41    3077.14    3082.73    3087.52
     8        3119.40    3114.19    3110.99    3102.97    3097.85    3094.21    3089.48    3085.84    3084.18    3085.28    3089.66    3094.02
     7        3119.40    3114.09    3109.30    3104.12    3100.40    3098.02    3095.84    3094.74    3095.31    3097.67    3101.28    3104.85
     6        3119.40    3114.01    3109.23    3105.34    3103.09    3102.51    3103.10    3104.97    3108.15    3112.24    3115.83    3118.64
     5        3119.40    3113.86    3109.33    3106.50    3105.88    3107.48    3110.89    3115.74    3121.48    3127.25    3131.76    3134.23
     4        3119.40    3113.33    3108.99    3107.24    3108.45    3112.47    3118.76    3126.59    3135.01    3142.83    3148.68    3151.41
     3        3119.40    3111.87    3107.55    3107.09    3110.40    3117.00    3126.15    3136.87    3147.98    3158.09    3165.74    3169.60
     2        3119.40    3108.20    3104.13    3105.58    3111.39    3120.62    3132.32    3145.44    3158.81    3171.12    3180.99    3187.15
     1        3119.40    3105.94    3102.63    3105.45    3112.28    3121.77    3132.94    3144.98    3157.18    3168.81    3179.08    3187.07
```

Exhibit VII-20 (Continued)

```
FILE NAME -- WIND              WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED                                  PAGE  2
WIND VELOCITIES   (IN METERS PER HOUR)  COMPONENT WINDY      VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195  6.00
 GRID CELL        13         14         15         16         17
     22      3109.38    3104.65    3103.30    3107.09    3119.40
     21      3107.72    3103.95    3103.60    3108.33    3119.40
     20      3106.23    3104.36    3105.66    3111.02    3119.40
     19      3107.51    3104.43    3106.53    3112.11    3119.40
     18      3101.76    3103.00    3106.54    3112.51    3119.40
     17      3100.65    3102.43    3106.46    3112.65    3119.40
     16      3100.28    3102.09    3106.34    3112.68    3119.40
     15      3100.35    3101.99    3106.29    3112.70    3119.40
     14      3101.00    3102.28    3106.41    3112.76    3119.40
     13      3100.44    3102.14    3106.37    3112.75    3119.40
     12      3098.46    3101.21    3105.91    3112.58    3119.40
     11      3094.44    3099.34    3105.00    3112.27    3119.40
     10      3090.97    3097.04    3104.09    3112.05    3119.40
      9      3092.24    3097.71    3104.85    3112.50    3119.40
      8      3098.26    3102.90    3108.25    3113.98    3119.40
      7      3108.07    3111.13    3113.63    3116.35    3119.40
      6      3120.16    3120.13    3119.94    3119.37    3119.40
      5      3133.91    3130.73    3127.52    3123.30    3119.40
      4      3150.19    3145.19    3138.15    3129.02    3119.40
      3      3168.74    3163.01    3152.85    3137.91    3119.40
      2      3188.54    3184.34    3173.40    3153.15    3119.40
      1      3191.59    3190.99    3182.66    3161.99    3119.40
```

Exhibit VII-20 (Concluded)

VIII SEGMENTATION OF M.E.B. FILES

If the entire modeling region is too large to fit within the core limitations of the Airshed Simulation Program, the region must be subdivided into rectangular subregions called "segments" that will fit into core. The segmentation process involves (1) determining the size and layout of the segments and (2) running the file segmentation program to create segmented versions of each spatially varying data file. This chapter first describes how to determine the core requirements for a given segmentation scheme and then how to use the file segmentation program.

A. CALCULATING CORE REQUIREMENTS

The maximum horizontal dimensions allowable for a single segment depend on the number of segments, the number of vertical levels and chemical species, and the number of point sources within the modeling region; the program options selected; and the amount of core available on the host computer. When the Airshed Simulation Program is installed on a particular computer, it will contain a vector of available space. The length of this vector is specified when the program is compiled and should be as large as possible. The vector of available space is used to hold the following four tables:

> Segment
> Local
> Boundary
> Segment scratch.

The detailed contents of these tables appear in Chapter VII of the Systems Manual. Only the methods of calculating the length of each table are described here.

To determine whether a segment of a given size will fit in core, the calculated sizes of the tables must be summed and that total compared with the amount of available core. The calculations for each table are discussed next, followed by Exhibit VIII-1, which is a worksheet to be used for the calculations. Finally, a sample problem is presented showing the calculation of core requirements for different segmentation schemes for the same region.

1. Segment Table

The Segment Table contains 65 entries for each segment.

$$S.T. = 65*seg \quad ,$$

where seg = number of segments.

2. Local Table

The Local Table contains vectors used by the numerical integration routines.

$$\begin{aligned} L.T. = 5 &+ 32z + zs + 5s \\ &+ 4r + 2r^2 \\ &+ 6x_{max} \quad , \end{aligned}$$

where

z = number of vertical levels,
s = number of chemical species,
r = number of reactive species,
x_{max} = maximum dimension in x or y direction for any segment.

Fixed Dimensions

z = ____
s = ____
r = ____

Simulation Options (1 = yes, 0 = no)

TEMPERATUR = ____
TERRAIN = ____
ROADWAY = ____
VARIATION = ____

	Segment			
	1	2	3	4
x				
y				
p				
interface				

$$65 \times \underset{\text{seg}}{\underline{\qquad}} = \underline{\qquad\qquad} \text{ (S.T.)}$$

$$\left[\begin{array}{l} 5 + \underset{32z}{\underline{\qquad}} + \underset{zs}{\underline{\qquad}} + \underset{5s}{\underline{\qquad}} \\ + \underset{4r}{\underline{\qquad}} + \underset{2r^2}{\underline{\qquad}} \\ + \underset{6(x,y)_{max}}{\underline{\qquad\qquad}} \end{array}\right] = \underline{\qquad\qquad} \text{ (L.T.)}$$

$$\left[\underset{8(x+y)}{\underline{\qquad}} + \underset{zs\ (interface)}{\underline{\qquad\qquad}} \right] = \underline{\qquad\qquad} \text{ (B.T.)}$$

$$\left[\begin{array}{l} 8 + \underset{2terr}{\underline{\qquad}} + \underset{temp}{\underline{\qquad}} + \underset{road}{\underline{\qquad}} \\ + \underset{2z}{\underline{\qquad}} \\ + \underset{S}{\underline{\qquad}} \left(2 + \underset{road}{\underline{\qquad}} + \underset{var}{\underline{\qquad}}\right) \\ + \underset{zs}{\underline{\qquad}} \end{array}\right] \begin{array}{l} \rightarrow \underset{[\ ]}{\underline{\qquad}} \times \underset{xy}{\underline{\qquad}} \\ \\ + \underset{2+s}{\underline{\qquad}} \times \underset{p}{\underline{\qquad}} = \underline{\qquad\qquad} \text{ (S.S.T.)} \end{array}$$

Sum of all tables = ________
Available storage = ________

Exhibit VIII-1. Storage Requirements Worksheet

3. Boundary Table

The Boundary Table contains the boundary cell definitions and the concentrations in the interface cells for a single segment. The "interface cells" of a segment are those that lie within the two-cell overlap into the adjacent segment. The number of interface cells in a segment is two times the sum of the lengths of each nonexternal edge. For nonsymmetrical segmentation schemes (such as that shown in Figure VIII-3), the Boundary Table length for each segment must be calculated to determine the maximum storage requirement.

$$\text{B.T.} = 8(x + y) + zs\,(\text{interface}) \quad ,$$

where

z = number of vertical levels,
s = number of chemical species,
$(x+y)$ = sum of x and y dimensions for the segment,
(interface) = number of interface cells in the segment, i.e., 2 times the length of all nonexternal edges.

4. Segment Scratch Table

The Segment Scratch Table contains all the other spatially varying data arrays, including predicted concentrations and variations, and the point source data, for one segment.

$$\begin{aligned}\text{S.S.T.} = xy \Big\{ & 8 + 2(\text{terr}) + 1\,(\text{temp}) + 1\,(\text{road}) \\ & + 2z + s[2 + 1(\text{road}) + 1(\text{var})] + zs \Big\} \\ & + p(2 + s) \quad ,\end{aligned}$$

where

x = number of cells in x direction;
y = number of cells in y direction;
p = number of point sources;
z = number of vertical levels;
s = number of chemical species;
terr = 1, if TERRAIN file input,
0, otherwise;
temp = 1, if TEMPERATUR file input,
0, otherwise;
road = 1, if ROADWAY file input,
0, otherwise;
var = 1, if concentration variations are calculated,
0, otherwise.

5. A Sample Problem

As an example, consider the region shown in Figure VIII-1, which is 17 x 22 cells, with the outer edge used as the boundary; the area modeled is thus 15 x 20 cells. There are 4 cells in the vertical direction, 13 chemical species to be modeled, and 200 elevated point sources. There are spatially varying terrain and temperature data but no roadway emissions file and, therefore, no surface layer variations. The core requirement calculations for this unsegmented region, which are shown in Exhibit VIII-2, indicate that the vector of available space must be at least 40373 words long. If it is not that long, the region must be divided into segments small enough to fit in core.

First, the user must try dividing the region in half, as shown in Figure VIII-2. (Recall that at each segment interface there is a two-cell overlap into the adjacent segment.) The resulting two segments are each 17 x 13 and the area modeled within each is 15 x 10. Each has one non-external edge 17 cells long. If the point sources are distributed fairly

Segment	Inner Area	Total Area	Interface Cells
1	15 x 20	17 x 22	0

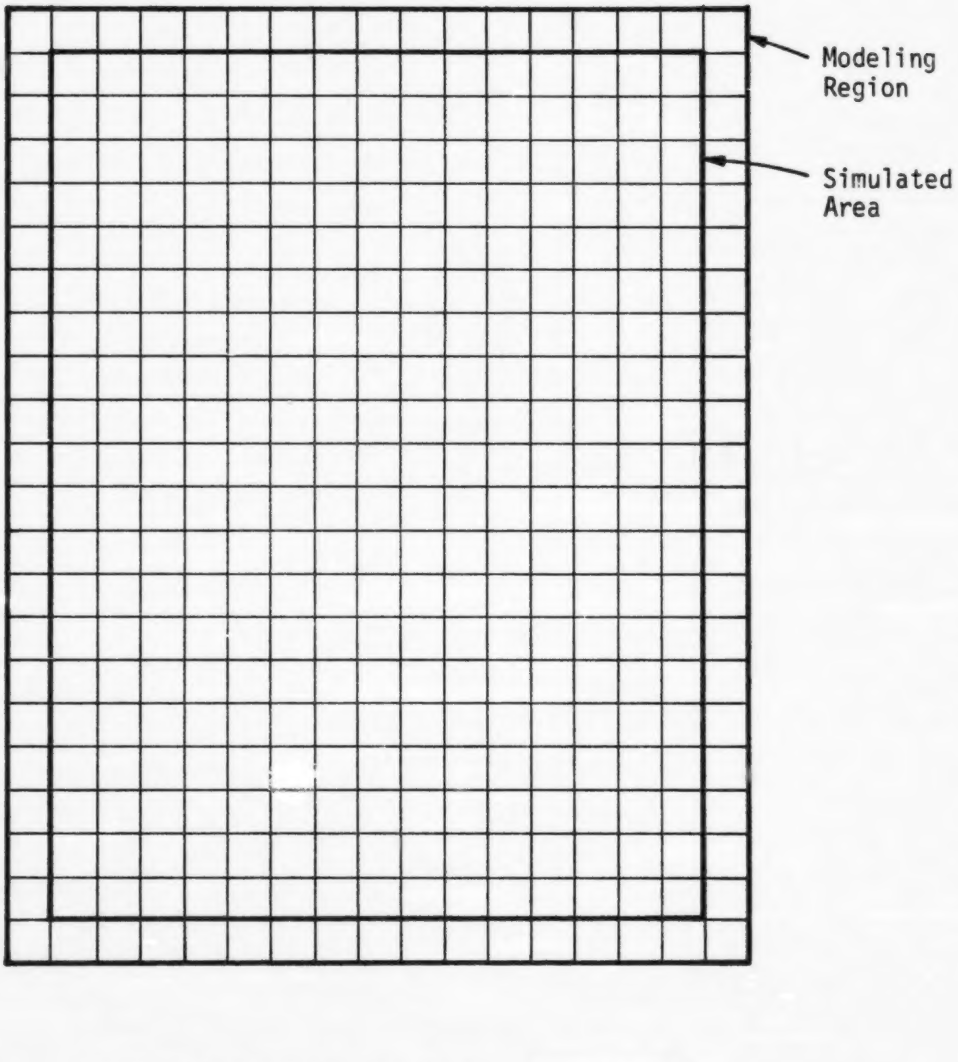

Modeling Region
Simulated Area

Figure VIII-1. Sample Region--Unsegmented

Fixed Dimensions

z = 4
s = 13
r = 12

Simulation Options (1 = yes, 0 = no)

TEMPERATUR = 1
TERRAIN = 1
ROADWAY = 0
VARIATION = 0

	Segment			
	1	2	3	4
x	17			
y	22			
p	200			
interface	–			

$65 \times \frac{1}{seg}$ = 65 (S.T.)

$$\left[5 + \frac{128}{32z} + \frac{52}{zs} + \frac{65}{5s} + \frac{48}{4r} + \frac{288}{2r^2} + \frac{132}{6(x,y)_{max}} \right]$$

= 718 (L.T.)

$$\left[\frac{8 \cdot 39}{8(x+y)} + \frac{0}{zs\ (interface)} \right]$$

= 312 (B.T.)

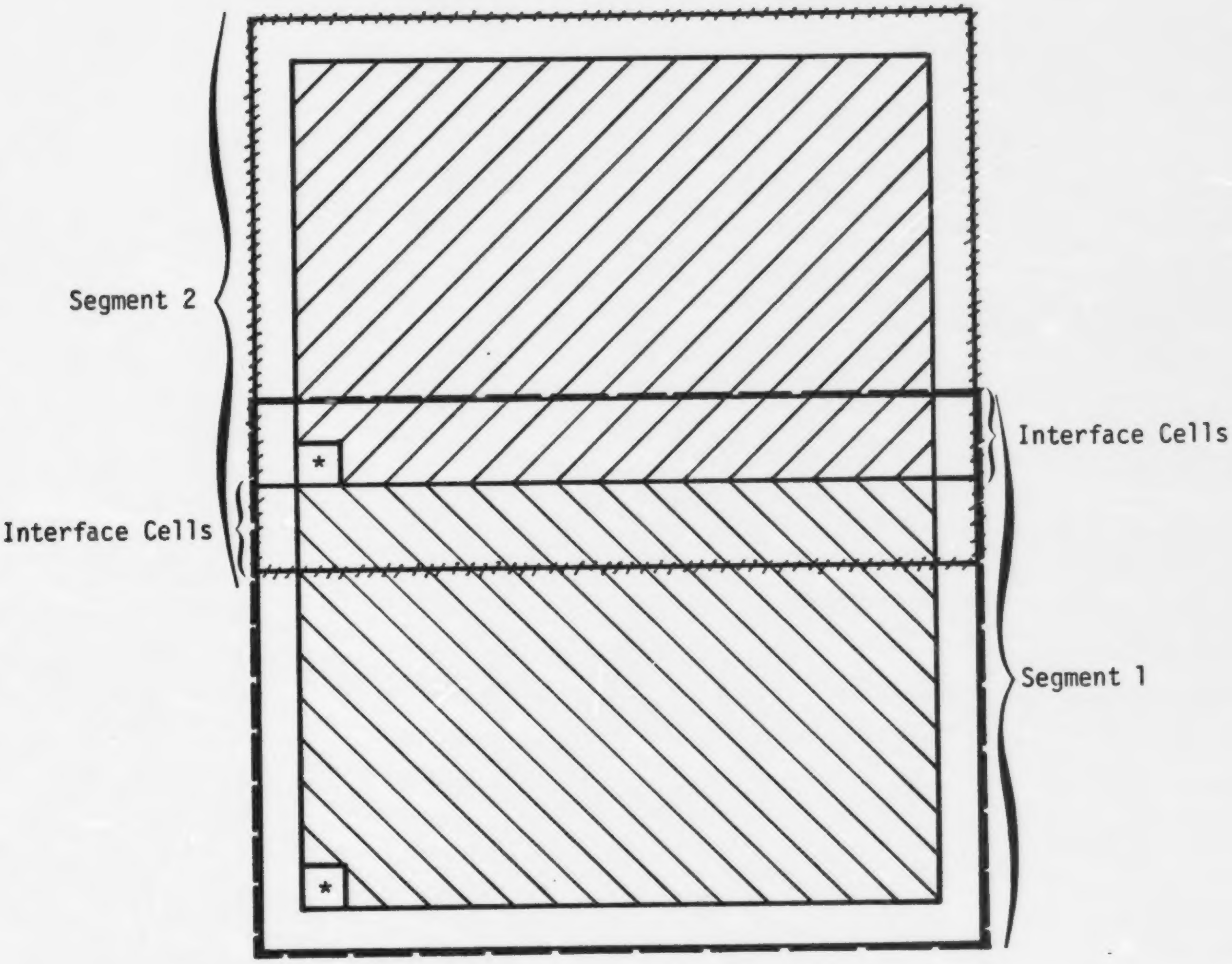
$$\left[8 + \frac{2}{2terr} + \frac{1}{temp} + \frac{0}{road} + \frac{8}{2z} + \frac{13}{S}\left(2 + \frac{0}{road} + \frac{0}{var}\right) + \frac{52}{zs} \right] \rightarrow \frac{97}{[\ ]} \times \frac{374}{xy}$$

$$+ \frac{15}{2+s} \times \frac{200}{p} =$$ 39278 (S.S.T.)

Sum of all tables = 40 373
Available storage = 30,000

Exhibit VIII-2. Worksheet Filled Out for an Unsegmented Region

Segment	Inner Area	Total Area	Interface Cells
1	15 x 10	17 x 13	2 x 17
2	15 x 10	17 x 13	2 x 17


Segment 2
Interface Cells
Interface Cells
Segment 1
*
*

* Segment origins input to the file segmentation program.

Figure VIII-2. Sample Region Divided into Two Segments

evenly throughout the region, there will be approximately 100 in each segment (count only the point sources within the modeled area, not those in the interface cells). Exhibit VIII-3 shows the computation of a core requirement of 25763 for this two-segment scheme.

If the two-segment scheme is still too large, the region can be further divided. Figure VIII-3 illustrates a three-segment scheme, without the actual segment edges drawn in. Size computations are shown in Exhibit VIII-4.

The objective of any segment layout design is to minimize the length of the segment boundaries to obtain segments that are as nearly square and equal sized as possible. Thus, the arrangement of the three segments shown in Figure VIII-3 represents a more efficient utilization of core space than that which would be obtained by merely cutting the region into three slices along either axis.

B. THE FILE SEGMENTATION PROGRAM

The spatially varying data files must be converted into segmented form according to the region segmentation scheme selected. If segmentation is not necessary, the files may be used in their unconverted form since unsegmented files are structured like segmented files that contain only one segment. The file segmentation program (SEGDEF) is used to create a segmented file from an unsegmented file. It will operate on any of the 11 spatially varying M.E.B. files, but only on one at a time. SEGDEF requires subroutines from the libraries UTILITY and FILUTIL.

The input to SEGDEF consists of a card deck and one unsegmented file, as illustrated in Figure VIII-4. The CONTROL and REGION packets are described in detail in Section V.A. The SEGMENTDEF and SEGMENT FILE packets are defined here in Sections B.1 and B.2.

Fixed Dimensions

z = 4
s = 13
r = 12

Simulation Options (1 = yes, 0 = no)

TEMPERATUR = 1
TERRAIN = 1
ROADWAY = 6
VARIATION = 0

Segment

	1	2	3	4
x	17	17		
y	13	13		
p	100	100		
interface	34	34		

$$65 \times \frac{2}{\text{seg}} = \underline{130}\ \text{(S.T.)}$$

$$\left[5 + \frac{128}{32z} + \frac{52}{zs} + \frac{65}{5s} + \frac{48}{4r} + \frac{288}{2r^2} + \frac{102}{6(x,y)_{\max}} \right] = \underline{688}\ \text{(L.T.)}$$

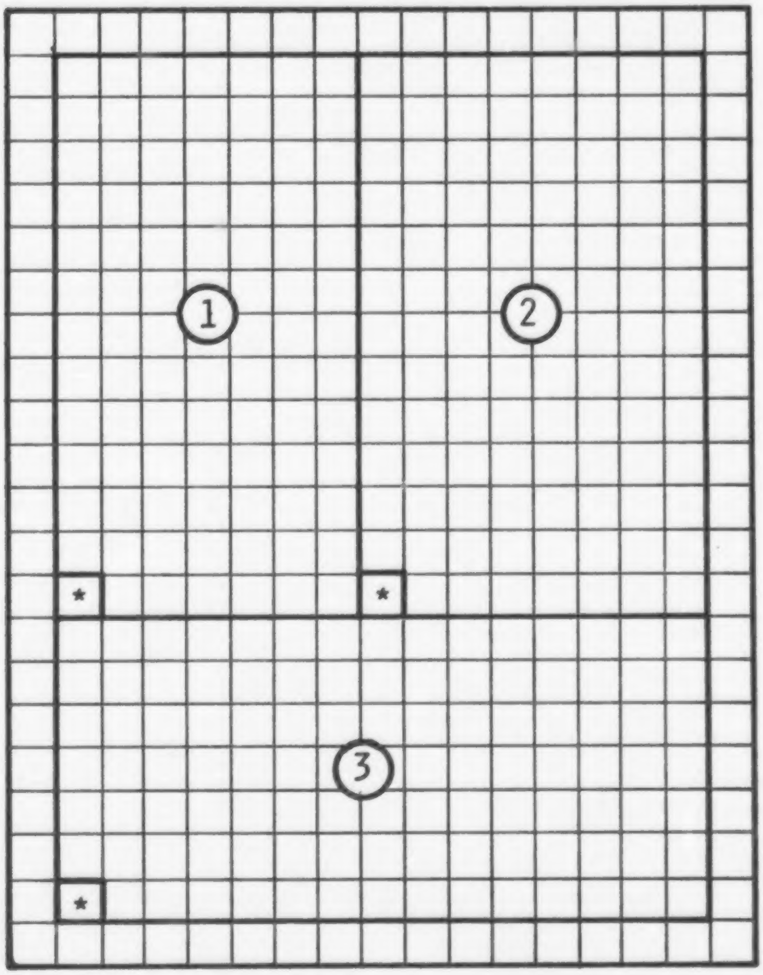
$$\left[\frac{240}{8(x+y)} + \frac{52 \cdot 34}{zs\ (\text{interface})} \right] = \underline{2008}\ \text{(B.T.)}$$

$$\left[8 + \frac{2}{2\text{terr}} + \frac{1}{\text{temp}} + \frac{0}{\text{road}} + \frac{8}{2z} + \frac{13}{S}\left(2 + \frac{0}{\text{road}} + \frac{0}{\text{var}}\right) + \frac{52}{zs} \right] \rightarrow \frac{97}{[\ ]} \times \frac{221}{xy} + \frac{15}{2+s} \times \frac{100}{p} = \underline{22937}\ \text{(S.S.T.)}$$

Sum of all tables = 25763
Available storage = 30000

Exhibit VIII-3. Worksheet Filled Out for a Two-Segment Region

Segment	Inner Area	Total Area	Interface Cells
1	7 x 13	10 x 16	2 x (10 + 16)
2	8 x 13	11 x 16	2 x (11 + 16)
3	15 x 7	17 x 10	2 x 17



* Segment origins input to the file segmentation program.

Figure VIII-3. Sample Region Divided into Three Segments

Fixed Dimensions

$z = 4$
$s = 13$
$r = 12$

Simulation Options (1 = yes, 0 = no)

TEMPERATUR = 1
TERRAIN = 1
ROADWAY = 0
VARIATION = 0

Segment

	1	2	3	4
x	10	11	17	
y	16	16	10	
p				
interface	52	54	34	

$$65 \times \frac{3}{\text{seg}} = 195 \text{ (S.T.)}$$

$$\left[5 + \frac{128}{32z} + \frac{52}{zs} + \frac{65}{5s} + \frac{48}{4r} + \frac{288}{2r^2} + \frac{102}{6(x,y)_{\max}}\right] = 688 \text{ (L.T.)}$$

$$\left[\frac{8 \cdot 27}{8(x+y)} + \frac{52 \cdot 54}{zs\ (\text{interface})}\right] = 3024 \text{ (B.T.)}$$

$$\left[8 + \frac{2}{2\text{terr}} + \frac{1}{\text{temp}} + \frac{0}{\text{road}} + \frac{8}{2z} + \frac{13}{S}\left(2 + \frac{-}{\text{road}} + \frac{-}{\text{var}}\right) + \frac{52}{zs}\right] \rightarrow \frac{97}{[\ ]} \times \frac{176}{xy} + \frac{15}{2+s} \times \frac{80}{p} = 18272 \text{ (S.S.T.)}$$

Sum of all tables = 22179
Available storage = 30000

Exhibit VIII-4. Worksheet Filled Out for a Three-Segment Region

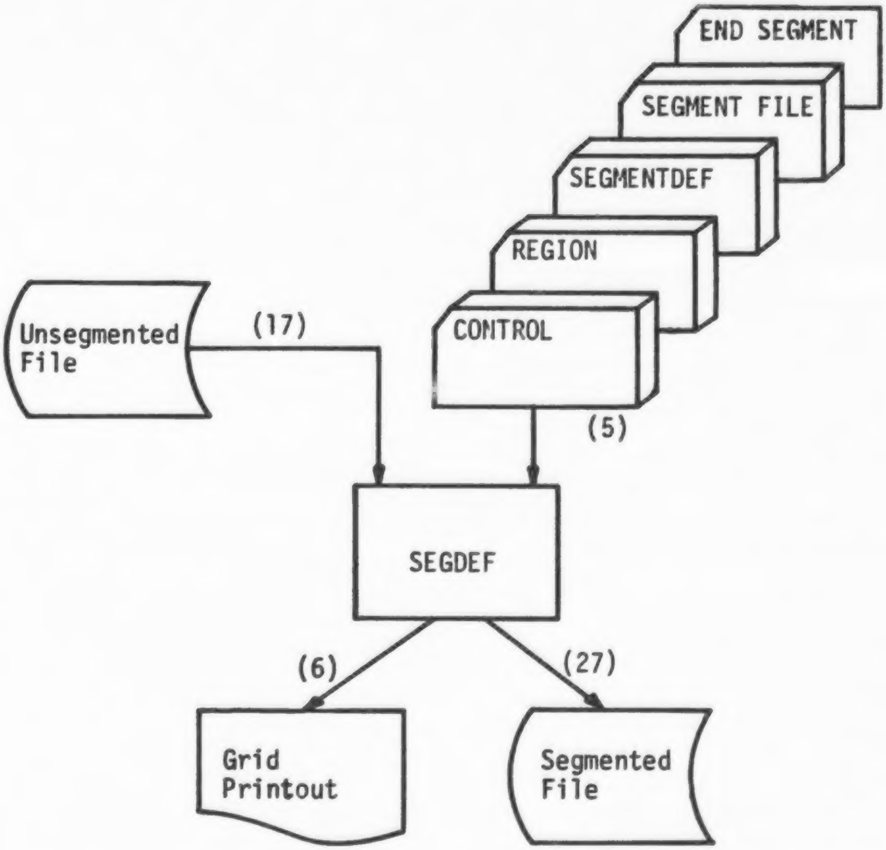

END SEGMENT
SEGMENT FILE
SEGMENTDEF
REGION
CONTROL
Unsegmented File
(17)
(5)
SEGDEF
(6)
(27)
Grid Printout
Segmented File

Figure VIII-4. Information Flow Diagram for the File Segmentation Program

The CONTROL packet entries for SEGDEF are shown in Table VIII-1. The following are special considerations for the CONTROL and REGION packets that pertain to this program:

- > CONTROL
    - The file name provided in Card 2 must be SEGMENTDEF.
    - The only options recognized by the file segmentation program are the number of species, the number of segments, and the print flags for the input cards and the segmented regional grid.
    - The beginning and ending dates can be the same as or contained within those of the file to be segmented.
    - The list of species may be a subset of the list in the file; their number must be the same as the entry in the control parameter above. If the file to be segmented contains no species, the list can be omitted.
- > REGION
    - This packet is standard in all respects. The region can be a subregion of the region described in the file; if the file is three-dimensional, vertical parameters in the REGION packet must match those on the file.

1. The SEGMENTDEF Packet

The SEGMENTDEF packet provides the definition of the segmentation scheme. The contents of this packet are described in Table VIII-2, and the format is shown in Exhibit VIII-5. For every segment there should be one Card 2 containing parameters defining the inner, modeled area of the grid. Thus, in the Figure VIII-2, a two-segment scheme, the origin of Segment 1 is defined as Cell (2,2) and its dimensions are 15 x 10. The origin of Segment 2 is defined as Cell (2,12) and its dimensions are also 15 x 10. The file segmentation program adds extra cells as necessary at external boundaries and at segment interfaces, and adjusts the origins and dimensions accordingly. In Figure VIII-3, the segment origins to be specified in the SEGMENTDEF packet are indicated by stars in the grid cells.

Table VIII-1. CONTROL Packet Entries for File Segmentation

Card Number	Entry
4	Number of species
	Spare
	Spare
	Number of segments
	Spare
	Spare
5	Spare
	Print input cards
	Print regional grid
	Spare
	Spare
	Spare
6	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
7	Spare
	Spare
	Spare
	Spare
	Spare
	Spare
8	Spare
	Spare
	Spare
	Spare
	Spare
	Spare

Table VIII-2. Contents of SEGMENTDEF Packet Cards

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be SEGMENTDEF, left adjusted
2+ Segment Definition	x-origin 1-10	I10	Grid units	x-index of cell in lower left corner of the modeled area of the segment
	y-origin 11-20	I10	Grid units	y-index of cell above
	Number of x-cells 21-30	I10	--	Length in x-direction of the modeled area of the segment
	Number of y-cells 31-40	I10	--	Length in y-direction of the modeled area of the segment
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	SEGMENTDEF						60A1
2+	Segment Definition	x-origin	y-origin	x-size	y-size			4I10
3	Packet Terminator	END						10A1

Exhibit VIII-5. SEGMENTDEF Packet Format

2. The SEGMENT FILE Packet

The SEGMENT FILE packet provides the name of the file to be segmented and the standard input and output units for the unsegmented and segmented files, respectively. The contents of this packet are described in Table I-3, and the format is shown in Exhibit VIII-6. The file name on the file designation card must be one of the following:

> AIRQUALITY
> BOUNDARY
> DIFFBREAK
> EMISSIONS
> PTSOURCE
> REGIONTOP
> ROADWAY
> TEMPERATUR
> TERRAIN
> TOPCONC
> WIND

The input file unit number must always be 17, and the output file unit number must always be 27.

Exhibit VIII-7 shows sample input to the file segmentation program; Exhibit VIII-8 shows sample output from this program.

Table VIII-3. Contents of SEGMENT FILE Packet Cards

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	60A1	--	Must be SEGMENT FILE, left adjusted
2 File Designation				
	File name 1-10	10A1	--	File name
	Input unit 11-20	I10	--	Unit number of unsegmented file--must be 17
	Output unit 21-30	I10	--	Unit number of segmented file--must be 27
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	SEGMENT FILE						60A1
2	File Designation	file name	input unit	output unit				10A1, 2I10
3	Packet Terminator	END						10A1

Exhibit VIII-6. SEGMENT FILE Packet Format

```
CONTROL
SEGMENT DEFINITION
SEGMENTATION OF ST. LOUIS FILES FOR 4 X 4 GRID
        11         0         0         2
                   1         1



NO
NO2
O3
ETH
OLE
PAR
CARB
ARO
BZA
PAN
CO
      76195       500     76195      2400
END
REGION
    725000.  4252000.         15
   -19000.   -16000.
      4000.     4000.
         17        22         4
          2         2      0.0        50.      200.
END
SEGMENTDEF
   1                2         2        15        10
   2                2        12        15        10
END
SEGMENT FILE
TEMPERATUR         17        27
END
```

Exhibit VIII-7. Sample Input to the File Segmentation Program

```
                                 REGIONAL DEFINITION

UTM ORIGIN X-COORDINATE                       725000.

UTM ORIGIN Y-COORDINATE                      4252000.

UTM ORIGIN ZONE NUMBER                             15

REGION ORIGIN X-COORDINATE                    -19000.

REGION ORIGIN Y-COORDINATE                    -16000.

CELL LENGTH IN X-DIRECTION                    4000.00

CELL LENGTH IN Y-DIRECTION                    4000.00

NUMBER OF CELLS IN X-DIRECTION                     17

NUMBER OF CELLS IN Y-DIRECTION                     22

NUMBER OF CELLS IN Z-DIRECTION                      4

NUMBER OF CELLS IN LOWER VERTICAL LAYER             2

NUMBER OF CELLS IN UPPER VERTICAL LAYER             2

HEIGHT OF SURFACE LAYER                           .00

MINIMUM CELL HEIGHT IN LOWER LAYER              50.00

MINIMUM CELL HEIGHT IN UPPER LAYER             200.00

KCRNT =    113  NSCLFT = 35798  IN SCRSET
KCRNT =    115  NSCLFT = 35796  IN SCRSET
KCRNT =    117  NSCLFT = 35794  IN SCRSET
KCRNT =    119  NSCLFT = 35792  IN SCRSET
KCRNT =    130  NSCLFT = 35781  IN SCRSET
KCRNT =    150  NSCLFT = 35761  IN SCRSET
KCRNT =    524  NSCLFT = 35387  IN SCRSET
SEGMENTDEF
  1               2         2        15        10
  2               2        12        15        10
END               0         0         0         0
```

Exhibit VIII-8. Sample output from the File Segmentation Program.

```
FILE NAME -- SEGMENTDEF     SEGMENTATION OF ST. LOUIS FILES FOR 4 X 4 GRID                                   PAGE  1

SEGMENT DEFINITION FOR DATA FILE CONTAINING,      SEGMENTDEF VERT.  LEVEL 1 START DATE/TIME 76195  5.00 STOP DATE/TIME 76195 24.00

 GRID CELL     1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16   17
     22        0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
     21        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     20        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     19        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     18        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     17        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     16        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     15        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     14        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     13        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     12        0    2    2    2    2    2    2    2    2    2    2    2    2    2    2    2    0
     11        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
     10        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      9        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      8        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      7        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      6        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      5        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      4        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      3        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      2        0    1    1    1    1    1    1    1    1    1    1    1    1    1    1    1    0
      1        0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
```

Exhibit VIII-8 (Continued)

```
                         SEGMENT DEFINITION TABLE

SEGMENT NAME   X-ORIGIN CELL  Y-ORIGIN CELL  NO. X-CELLS    NO. Y-CELLS


1                          0              0           17             13

2                          0              9           17             13

SEGMENT FILE
TEMPERATUR        17        27
KCRNT =    375  NSCLFT = 35013  IN SCRSET
KCRNT =    749  NSCLFT = 34639  IN SCRSET
KCRNT =   1123  NSCLFT = 34265  IN SCRSET
END                0         0
```

Exhibit VIII-8 (Continued).

```
PROCESSING OF INPUT DATA FOR THE PREPARATION OF FILE SEGMENTDEF

SEGMENTATION OF ST. LOUIS FILES FOR 4 X 4 GRID

NUMBER OF SPECIES =         11

NUMBER OF SEGMENTS =          2

INPUT CARDS WILL BE PRINTED

BEGINNING DATE OF FILE      76195 BEGINNING TIME OF FILE       5.00

ENDING DATE OF FILE      76195 ENDING TIME OF FILE      24.00

A TOTAL OF         11 SPECIES NAMES WERE READ ,

THE SPECIES NAMES ARE --

NO

NO2

O3

ETH

OLE

PAR

CARB

ARO

BZA

PAN

CO

REGION
   725000.  4252000.        15
   -19000.   -16000.
   4000.00   4000.00
        17        22         4
         2         2       .00     50.00    200.00
END
```

Exhibit VIII-8 (Concluded).

IX PREPARATION OF CONTROL DATA

Of the 14 files input to the Airshed Simulation Program, two are classified as control data files: the Chemistry Parameters file (CHEMPARAM), and the Simulation Controls file (SIMCONTROL). This chapter describes in detail the preparation of these files and includes for each a job control illustration, packet item definitions and packet formats, worksheets, and sample input and output listings.

A. THE CHEMISTRY PARAMETERS FILE

The Chemistry Parameters (CHEMPARAM) file names the species to be simulated and specifies values for species-related and reaction-related parameters. Figure IX-1 is an information flow diagram for use in setting up the job control for a CHEMPARAM file creation run. The program that creates the CHEMPARAM file is called CPREP; it requires as input a CONTROL packet, a SPECIES packet, and if there is to be chemistry, a REACTIONS packet and a COEFFICIENTS packet (fully described below). The printed output from CPREP consists of input numbers, error messages, if any, and the values written to the CHEMPARAM file (see Section A.5 of this chapter for sample input and output listings). The file itself is written to FORTRAN Unit 2, and the file format is given in Chapter IX of the Systems Manual.

1. CONTROL Packet Rules for the CHEMPARAM File

An abbreviated CONTROL packet is used to create the CHEMPARAM file. The packet names and identifies the file and specifies for it the number of species, reactions, and coefficients. This packet must be entered before any other packet. The contents of each card in the CONTROL packet are described in Table IX-1 and the format is shown in Exhibit IX-1.

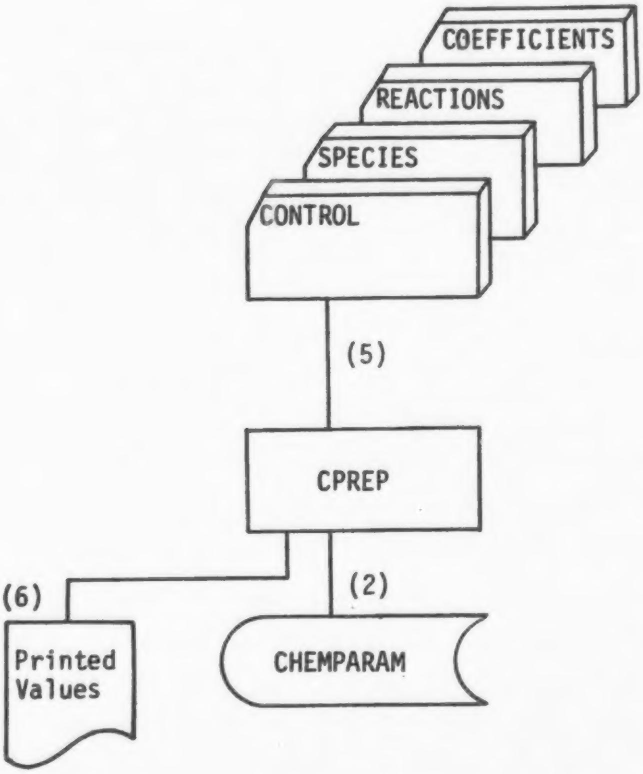

COEFFICIENTS
REACTIONS
SPECIES
CONTROL
(5)
CPREP
(6)
(2)
Printed Values
CHEMPARAM

Figure IX-1. Information Flow Diagram for Use in Creation of the CHEMPARAM File

Table IX-1. CONTROL Packet for the CHEMPARAM File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	10A1	--	Must be CONTROL, left adjusted
2 File Name	File name 1-10	10A1	--	Must be CHEMPARAM, left adjusted
3 File Identifier	Identifier 1-60	60A1	--	Any 60 characters; the file identifier will appear on the File Description Header Record
4 Control Options				
	Number of species 1-10	I10	--	Must be at least 1; the number of species that will appear in the SPECIES packet and that will thus be included in the airshed simulation; at present, this number must be $\leq$ 20
	Number of reactions 11-20	I10	--	The number of reactions that will be described in the REACTIONS packet; for the Carbon-Bond Mechanism, this number should be 69; at present, this number must be $\leq$80.
	Number of coefficients 21-30	I10	--	The number of coefficients that will be defined in the COEFFICIENTS packet; if inert species only are to be simulated, set this number to zero and omit the COEFFICIENTS packet; for the Carbon-Bond Mechanism, this number should be 4; at present, this number must be $\leq$10
5 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	CONTROL						10A1
2	File Name	CHEMPARAM						10A1
3	File Identifier							60A1
4	Control Parameters	# species	# reacs	# coeffs				3I10
5	Packet Terminator	END						10A1

Exhibit IX-1. CONTROL Packet Format for the CHEMPARAM File

2. SPECIES Packet Rules for the CHEMPARAM File

The SPECIES packet must follow the CONTROL packet in the input deck used to create the CHEMPARAM file. The SPECIES packet consists of a packet header card, one pair of Cards 2 and 3 for each species to be simulated, and a packet terminator card. The contents of each card in the SPECIES packet are described in Table IX-2, and the format is shown in Exhibit IX-2.

The chemical species can appear in any order on the CHEMPARAM file, provided that all the reactive species precede all the unreactive species. The output files AVERAGE, INSTANT, and VARIATION will contain these species in this order.

If any reactive species are to be simulated, their names must correspond to the species names used in the chemical mechanism that is built into the program. For the Carbon-Bond II Mechanism (currently built into the program), the following species names are required:

> NO
> NO2
> O3
> ETH
> OLE
> PAR
> CARB
> ARO
> BZA
> PAN
> CO.

All the first 10 species (NO through PAN) must appear (though not necessarily in the order listed) and all must be flagged as reactive. CO must

Table IX-2. SPECIES Packet for the CHEMPARAM File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	10A1	--	Must be SPECIES, left adjusted
Species Name and Flags				
	Species name 1-10	10A1	--	Any 10-characters, left adjusted
	Reactive flag 11	A1, 9X	--	An R in Col. 11 indicates that the species is reactive; anything else means unreactive
	Steady-state initial conditions flag 30	9X, L1	--	T or F in Col. 30--a blank means false; if true, steady-state computations will be performed in the Airshed Simulation Program to set initial concentrations; at present, these computations are implemented in the Carbon-Bond Mechanism for O_3 only; when computations are performed for O_3, concentrations of NO and NO_2 are also adjusted
	Steady-state boundary conditions flag 40	9X, L1	--	T or F in Col. 40--a blank means false; if true, steady-state computations will be performed at each time slice in the airshed simulation to set boundary concentrations on the vertically varying west, east, south, and north planes (from file BOUNDARY) and on the x-y plane at the top of the region (from file TOPCONC); at present, these computations are implemented in the Carbon-Bond Mechanism for O_3 only; when computations are performed for O_3, concentrations of NO and NO_2 are also adjusted

Table IX-2 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
3 Other Parameters				
	Surface uptake resistance 1-10	F10.0	$(m/hr)^{-1}$	To eliminate surface deposition, set this number to a high value, e.g., 1.E6
	Steady-state lower bound 11-20	F10.0	ppm ($\mu g/m^3$ for AEROSOLS)	Computed steady-state concentrations will not be allowed to go below this value, which will also be used for initial or boundary concentrations if this species is missing from an input data file (AIRQUALITY, BOUNDARY, or TOPCONC)
	Steady-state upper bound 21-30	F10.0	ppm ($\mu g/m^3$ for AEROSOLS)	This number must be greater than the steady-state lower bound; computed steady-state concentrations will not be allowed to exceed this value.
	Numerical lower bound 31-40	F10.0	ppm ($\mu g/m^3$ for AEROSOLS)	Computed concentrations will not be allowed to go below this value in the horizontal transport steps of the simulation
	Numerical upper bound 41-50	F10.0	ppm ($\mu g/m^3$ for AEROSOLS)	This number must be greater than the numerical lower bound; computed concentrations will not be allowed to exceed this value in the horizontal transport steps of the simulation (at present, this test is not implemented)
4 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	SPECIES						10A1
2	Species Name and Flags	species name	reactive	st-st i conc	st-st b conc			10A1, A1, 9X, 2L10
3	Other Species Parameters	surf uptake resis	low bd st-st	up bd st-st	low bd num	up bd num		5F10.0
4	Packet Terminator	END						10A1

Exhibit IX-2. SPECIES Packet Format for the CHEMPARAM File

also appear, without a reactive flag, and must follow the listing of all the reactive species. SO2 and AEROSOLS each can be named as reactive or unreactive, or they can be omitted from the simulation altogether. Any other reactive species are illegal, since there have been no reactions defined to deal with them. However, any other unreactive species can be specified without limitation other than core availability.

The species names on the species-varying data files must also correspond to the names in the CHEMPARAM file. If a name that is not on the CHEMPARAM file appears on a data file, the data for that species will be ignored. If a name is on the CHEMPARAM file but does not appear on a data file, the following default values apply:

- For concentration data (from AIRQUALITY, BOUNDARY, or TOPCONC), the steady-state lower bound values (see Card 3 of the SPECIES packet) will be used.
- For emissions data (from EMISSIONS, ROADWAY, or PTSOURCE), the value zero will be used.

Exhibit IX-3(a) is a worksheet that can be used to aid in the preparation of the SPECIES packet. Exhibit IX-3(b) is a sample of that worksheet filled in with typical values used for the Carbon-Bond II Mechanism.

Species	Reactive?	Steady-State Initial	Steady-State Boundary	Surface Uptake Resistance	Steady-State Lower Bound	Steady-State Upper Bound	Numerical Lower Bound	Numerical Upper Bound
	11	21-30	31-40	1-10	11-20	21-30	31-40	41-50
	A1	L10	L10	F10.0	F10.0	F10.0	F10.0	F10.0

(a) Format

Exhibit IX-3. SPECIES Definition Worksheet

Species	Reactive?	Steady-State Initial	Steady-State Boundary	Surface Uptake Resistance	Steady-State Lower Bound	Steady-State Upper Bound	Numerical Lower Bound	Numerical Upper Bound
Col	11	21-30	31-40	1-10	11-20	21-30	31-40	41-50
For	A1	L10	L10	F10.0	F10.0	F10.0	F10.0	F10.0
NO	R	F	F	0.28	1. E-5	1. E+6	1. E-5	1. E+6
NO2	R	F	F	0.0111	1. E-4		1. E-4	
O3	R	T	T	0.0147	1. E-7		1. E-7	
ETH	R	F	F	1. E+10	1. E-4		1. E-4	
OLE	R	F	F	1. E+10	1. E-4		1. E-4	
PAR	R	F	F	1. E+10	1. E-4		1. E-4	
CARB	R	F	F	1. E+10	1. E-4		1. E-4	
ARO	R	F	F	1. E+10	1. E-4		1. E-4	
PAN	R	F	F	1. E+10	1. E-8		1. E-8	
BZA	R	F	F	1. E+10	1. E-8		1. E-8	
AEROSOLS	R	F	F	1. E+10	24.0		24.0	
SO2	R	F	F	.0097	1. E-6		1. E-6	
CO	U	F	F	1. E+10	0.01		0.01	

(b) Worksheet Filled In with Typical Values Used for the Carbon-Bond II Mechanism

Exhibit IX-3 (Concluded)

3. REACTIONS Packet Rules for the CHEMPARAM File

If the number of reactions specified in the CONTROL packet is greater than zero, there must be a REACTIONS packet following the SPECIES packet. If there are no reactions, the REACTIONS packet must be omitted. This packet consists of a header card, a mechanism name, one card for each reaction, and a packet terminator. The contents of each card in the REACTIONS packet are listed in Table IX-3, and the format is shown in Exhibit IX-4.

For simulation purposes, a reaction is considered to be photolysis, or temperature-dependent, or neither of these. If the photolysis flag is "on" (i.e., a value of P is punched in Column 21), the reaction is photolysis. If the photolysis field is not P and the reaction rate constant and activation energy are nonzero, the reaction is temperature-dependent, and a nonzero value for the reference temperature must be provided. If the reaction rate constant or the activation energy is zero, the reaction is considered to be not temperature dependent. Exhibit IX-5(a) is a worksheet that can be used to aid in the preparation of the REACTIONS packet. Exhibit IX-5(b) is a sample of that worksheet filled in with typical values used for the Carbon-Bond II Mechanism. Since temperature-dependent reaction rates are recalculated with an exponential expression at each time step in each grid cell, it is suggested that the temperature-dependence parameters--activation energy and reference temperatures--be specified for only those reactions for which the temperature range experienced during the simulation period will produce significant differences in predicted concentrations. For the Carbon-Bond Mechanism, the activation energies considered important at present are indicated in the example of Exhibit IX-5(b).

Table IX-3. REACTIONS Packet for the CHAMPARAM File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	10A1	--	Must be REACTIONS, left adjusted
2 Mechanism Name	Mechanism name 1-60	60A1	--	Any 60-character string; this name will appear in the file and on any simulation runs using the file
3 Reaction Parameters				Must be 1 card for each reaction
	Reaction number 1-10	I10	--	This number is used to place the reaction parameters in their respective vectors, as well as to aid in visual identification; although the scheme described allows reaction parameter cards to appear in any sequence, strict adherence to numerical order is suggested to avoid omission or duplication of reactions
	Nominal reaction rate constant 11-20	F10.0	ppm^{-n} hours^{-1}* for nonphotolysis reactions	For photolysis reactions, this number is multiplied by the parameter RADFACTOR on the METSCALARS file (see Chapter VII on METSCALARS); RADFACTOR is the NO_2 photolysis rate constant expressed in min^{-1}; therefore, this number is not a rate constant but rather is a dimensionless factor for relating each photolysis rate constant to the temporally varying NO_2 photolysis rate constant and for converting the rate from min^{-1} to hour^{-1}

Table IX-3. (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
3 (cont'd)				
	Reaction type 21	A1, 9X	--	If Col. 21 is set to P, it will be considered a photolysis reaction
	Activation energy 31-40	F10.0	°K	If this field is left blank, temperature dependence calculations will not be performed
	Reference temperature 41-50	F10.0	°K	This field must be set to nonzero if both the reaction rate and the activation energy are nonzero
4 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

---

* The value of n is determined by the order of the reaction. For example, n takes on values of 0, 1, and 2 for first-, second-, and third-order reactions, respectively.

Card Number	Card Identifier	1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	REACTIONS						10A1
2	Mechanism Name							60A1
3	Reaction Parameters	reac #	rate const	type	act energy	ref temp		I10, F10.0, A1, 9X, 2F10.0
4	Packet Terminator	END						10A1

Exhibit IX-4. REACTIONS Packet Format for the CHEMPARAM File

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0

(a) Format

Exhibit IX-5. REACTIONS Definition Worksheet

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0
	$NO_2 + h\nu \rightarrow NO + O$	1	60.	P		
	$O \xrightarrow{O_2 + M} O_3$	2	2.64E + 8			
	$O_3 + NO \rightarrow NO_2 + O_2$	3	1.434E + 3		1450.	298.
	$O_3 + NO_2 \rightarrow NO_3 + O_2$	4	2.88		2450.	298.
	$O + NO_2 \rightarrow NO + O_2$	5	8.04E + 5			
	$O_3 + OH \rightarrow HO_2 + O_2$	6	4.62E + 3		1000.	298.
	$O_3 + HO_2 \rightarrow OH + 2O_2$	7	3.00E + 2		1525.	298.
	$NO_2 + OH \rightarrow HNO_3$	8	8.40E + 5			
	$CO + OH \xrightarrow{O_2} HO_2 + CO_2$	9	2.64E + 4			
	$NO + NO \xrightarrow{O_2} 2NO_2$	10	9.00E - 3			
	$NO_3 + NO \rightarrow 2NO_2$	11	1.68E + 6			

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0
	$NO_3 + NO_2 + H_2O \rightarrow 2HNO_3$	12	9.00E - 3		-10600.	298.
	$HO_2 + NO \rightarrow NO_2 + OH$	13	7.20E + 5			
	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	14	9.00E + 5			
	$PAR + O \rightarrow MEO_2 + OH$	15	1.20E + 3			
	$PAR + OH \rightarrow MEO_2$	16	9.00E + 4			
	$OLE + O \rightarrow MEO_2 + ACO_3 + X$	17	1.62E + 5			
	$OLE + O \rightarrow CARB + PAR$	18	1.62E + 5			
	$OLE + OH \rightarrow RAO_2$	19	2.52E + 6			
	$OLE + O_3 \rightarrow CARB + CRIG$	20	4.80E - 1			
	$OLE + O_3 \rightarrow CARB + MCRG + X$	21	4.80E - 1			
	$ETH + O \rightarrow MEO_2 + HO_2 + CO$	22	3.60E + 4			
	$ETH + O \rightarrow CARB + PAR$	23	3.60E + 4			
	$ETH + OH \rightarrow RBO_2$	24	7.20E + 5			

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0
	ETH + O_3 → CARB + CRIG	25	1.44E - 1			
	ACO_3 + NO → NO_2 + MEO_2 + CO_2	26	2.28E + 5			
	RBO_2 + NO → NO_2 + 2 CARB + HO_2	27	7.20E + 5			
	RAO_2 + NO → NO_2 + 2 CARB + HO_2	28	7.20E + 5			
	MEO_2 + NO → NO_2 + CARB + MEO_2 + X ·	29	2.30E + 5			
	MEO_2 + NO → NO_2 + CARB + HO_2	30	4.60E + 5			
	MEO_2 + NO → Nitrates	31	3.00E + 4			
	RBO_2 + O_3 → 2 CARB + HO_2	32	3.00E + 2			
	RAO_2 + O_3 → 2 CARB + HO_2	33	1.20E + 4			
	MEO_2 + O_3 → CARB + HO_2	34	3.00E + 2			
	CARB + OH → α (HO_2 + CO) + (1 - α) (ACO_3 + X)	35	1.14E + 6			
	CARB + $h\nu$ → CO	36	1.35E - 3	P		
	CARB + $h\nu$ → (1 + α) HO_2 + (1 - α) (MEO_2 + X) + CO	37	1.215E - 1	P		

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0
	X + PAR → Products	38	6.00E + 6			
	ACO$_3$ + NO$_2$ → PAN	39	1.20E + 5			
	PAN → ACO$_3$ + NO$_2$	40	1.68E + 0		12500.	298.
	ACO$_3$ + HO$_2$ → Products	41	2.40E + 5			
	MEO$_2$ + HO$_2$ → Products	42	2.40E + 5			
	CRIG + NO → NO$_2$ + CARB	43	7.20E + 5			
	CRIG + NO$_2$ → NO$_3$ + CARB	44	4.80E + 5			
	CRIG + CARB → Ozonide	45	1.20E + 5			
	MCRG + NO → NO$_2$ + CARB + PAR	46	7.20E + 5			
	MCRG + NO$_2$ → NO$_3$ + CARB + PAR	47	4.80E + 5			
	MCRG + CARB → Ozonide	48	2.00E + 3			
	CRIG → CO	49	4.02E + 4			
	CRIG → Products	50	1.44E + 4			

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0
	$CRIG \rightarrow 2HO_2 + CO_2$	51	5.40E + 3			
	$MCRG \rightarrow$ Products	52	9.00E + 3			
	$MCRG \rightarrow MEO_2 + OH + CO$	53	2.04E + 4			
	$MCRG \rightarrow MEO_2 + HO_2 + CO_2$	54	2.55E + 4			
	$MCRG \rightarrow CARB + 2HO_2 + CO$	55	5.10E + 3			
	$ARO + OH \rightarrow HO_2 + 3\ ARPI$	56	3.60E + 5			
	$ARO + OH \rightarrow HO_2 + BZA + X$	57	9.60E + 4			
	$ARO + OH \rightarrow OH + BZA + W$	58	9.00E + 5			
	$CARB + W \rightarrow$ Products	59	6.00E + 6			
	$NO + ARPI \rightarrow PAR + CARB + NO$	60	1.80E + 3			
	$NO + ARPI \rightarrow NO_2 +$ Aerosol	61	9.00E + 2			
	$NO_3 + ARPI \rightarrow 2\ CARB$	62	2.10E + 6			

	Reaction	Number	Rate Constant	Type	Activation Energy	Reference Temperature
Column		1-10	11-20	21	31-40	41-50
Format		I10	F10.0	A1	F10.0	F10.0
	$O_3 + APRI \rightarrow Aerosol$	63	3.60E + 1			
	$BZA + OH \rightarrow HO_2 + CO + 3\ ARPI$	64	6.00E + 5			
	$BZA \rightarrow MEO_2 + HO_2 + 3\ ARPI$	65	2.16E + 0	P		
	$SO_2 + OH \xrightarrow{O_2} HSO_5$	66	5.40E + 1			
	$HSO_5 + NO \rightarrow NO_2 + HSO_4$	67	4.80E + 4			
	$HSO_4 + NO_2 \rightarrow H_2SO_4 + HNO_3$	68	5.40E + 5			
	$SO_2 \rightarrow Aerosol$	69	3.00E - 2			

4. COEFFICIENTS Packet Rules for the CHEMPARAM File

If the number of coefficients specified in the CONTROL packet is greater than zero, there must be a COEFFICIENTS packet, and it must follow the REACTIONS packet (or the SPECIES packet, if there is no REACTIONS packet). If there are no coefficients, this packet must be omitted. The COEFFICIENTS packet consists of a header card, one card for each coefficient, and a packet terminator. The contents of each card are described in Table IX-4, and the format is shown in Exhibit IX-6.

Exhibit IX-7(a) is a worksheet that can be used to aid in the preparation of the COEFFICIENTS packet. Exhibit IX-7(b) is a sample of that worksheet filled in with typical values used for the Carbon-Bond II Mechanism.

Table IX-4. COEFFICIENTS Packet for the CHEMPARAM File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	10A1	--	Must be COEFFICIENTS, left adjusted
2 Coefficient				
	Coefficient name 1-10	10A1	--	10 characters, left adjusted; must be identical to a coefficient name required by the built-in chemical mechanism
	Coefficient value 11-20	F10.0	--	
3 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	COEFFICIENTS						10A1
2	Coefficients	Name	Value					10A1, F10.0
3	Packet Terminator	END						10A1

Exhibit IX-6. COEFFICIENTS Packet Format for the CHEMPARAM File

	Meaning	Name	Value
Column		1-10	11-20
Format		10A1	F10.0

(a) Format

Exhibit IX-7. COEFFICIENTS Definition Worksheet

	Meaning	Name	Value
Column		1-10	11-20
Format		10A1	F10.0
		ALPHA	0.5
		BETA	.48
		GAMMA	1.0
		ETA	0.1

(b) Worksheet Filled In with Typical Values Used for the Carbon-Bond Mechanism

Exhibit IX-7 (Concluded)

5. CPREP Sample Input and Output

Exhibit IX-8 is a listing of an input deck used to create a CHEMPARAM file; it contains the values from the sample worksheets [Exhibits IX-3(b), IX-5(b), and IX-7(b)]. Exhibit IX-9 is the printout that was generated by CPREP; the first two pages list the values on the input cards as they are read in, and the last two show the values put out to the CHEMPARAM file.

```
CONTROL
CHEMPARAM
  CHEMISTRY PARAMETERS  NEW CHEM  HIGHER PARAFINS LOWER LIMIT
        11         69          4
END
SPECIES
NO          R          F          F
     0.28     1.0E-5     1.0E+6     1.0E-5     1.0E+6
NO2         R          F          F
    0.0111     1.E-4      1.E+6      1.E-4      1.E+6
O3          R          T          T
    0.0147     1.E-9      1.E+6      1.E-9      1.E+6
ETH         R          F          F
     1.E10     1.E-6      1.E+6      1.E-6      1.E+6
OLE         R          F          F
     1.E10     1.E-6      1.E+6      1.E-6      1.E+6
PAR         R          F          F
     1.E10     1.E-3      1.E+6      1.E-4      1.E+6
CARB        R          F          F
     1.E10     1.E-6      1.E+6      1.E-6      1.E+6
ARO         R          F          F
     1.E10     1.E-6      1.E+6      1.E-6      1.E+6
BZA         R          F          F
     1.E10     1.E-6      1.E+6      1.E-6      1.E+6
PAN         R          F          F
     1.E10     1.E-6      1.E+6      1.E-6      1.E+6
CO          R          F          F
     1.E10       .01      1.E+6        .01      1.E+6
END
REACTIONS
CARBON BOND MECHANISM -- NOVEMBER 78
         1  60.00E+0P
         2   264.E+6
         3 1434.                    1450.      298.
         4   288.E-2                2450.      298.
         5   80.4E+4
         6   462.E+1                1000.      298.
         7  300.                    1525.      298.
         8    84.E+4
         9   264.E+2
        10    90.E-4
        11   168.E+4
        12    9.0E-3               -10600.     298.
        13    72.E+4
        14    90.E+4
        15   120.E+1
        16    90.E+3
        17   162.E+3
        18   162.E+3
        19   252.E+4
        20   480.E-3
        21   480.E-3
        22   360.E+2
        23   360.E+2
        24    72.E+4
```

Exhibit IX-8. Sample CPREP Input for the CHEMPARAM File

```
      25   144.E-3
      26   228.E+3
      27    72.E+4
      28    72.E+4
      29    2.3E+5
      30    4.6E+5
      31   300.E+2
      32  300.
      33   120.E+2
      34  300.
      35   114.E+4
      36    81.E-3P
      37  121.5E-3P
      38    60.E+5
      39   120.E+3
      40   168.E-2               12500.     298.
      41   240.E+3
      42   240.E+3
      43    72.E+4
      44   480.E+3
      45   120.E+3
      46    72.E+4
      47   480.E+3
      48   120.E+3
      49   402.E+2
      50   144.E+2
      51   540.E+1
      52    90.E+2
      53   204.E+2
      54   255.E+2
      55   510.E+1
      56   3.60E+5
      57    9.6E+4
      58    9.0E+5
      59    6.0E+6
      60    1.8E+3
      61    9.0E+2
      62    2.1E+6
      63    3.6E+1
      64    6.0E+5
      65  2.160E+0P
      66 540.00E+2
      67 480.00E+2
      68 540.00E+3
      69   3.00E-2
END
COEFFICIENTS
ALPHA            0.5
BETA             .48
GAMMA            1.0
ETA              0.1
END
```

Exhibit IX-8 (Concluded)

```
CONTROL
CHEMPARAM
  CHEMISTRY PARAMETERS  NEW CHEM  HIGHER PARAFINS LOWER LIMI
      11         69         4
END
SPECIES
NO         R                  F          F
     2.8000-001    1.0000-005    1.0000+006    1.0000-005    1.0000+006
NO2        R                  F          F
     1.1100-002    1.0000-004    1.0000+006    1.0000-004    1.0000+006
O3         R                  T          T
     1.4700-002    1.0000-009    1.0000+006    1.0000-009    1.0000+006
ETH        R                  F          F
     1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
OLE        R                  F          F
     1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
PAR        R                  F          F
     1.0000+010    1.0000-003    1.0000+006    1.0000-004    1.0000+006
CARB       R                  F          F
     1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
APO        R                  F          F
     1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
BZA        R                  F          F
     1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
PAN        R                  F          F
     1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
CO         R                  F          F
     1.0000+010    1.0000-002    1.0000+006    1.0000-002    1.0000+006
END
REACTIONS
CARBON BOND MECHANISM -- NOVEMBER 78
         1     6.0000+001  P              .0000          .0000
         2     2.6400+008                 .0000          .0000
         3     1.4340+003             1.4500+003     2.9800+002
         4     2.8800+000             2.4500+003     2.9800+002
         5     8.0400+005                 .0000          .0000
         6     4.6200+003             1.0000+003     2.9300+002
         7     3.0000+002             1.5250+003     2.9800+002
         8     8.4000+005                 .0000          .0000
         9     2.6400+004                 .0000          .0000
        10     9.0000-003                 .0000          .0000
        11     1.6800+006                 .0000          .0000
        12     9.0000-003            -1.0600+004     2.9800+002
        13     7.2000+005                 .0000          .0000
        14     9.0000+005                 .0000          .0000
        15     1.2000+003                 .0000          .0000
        16     9.0000+004                 .0000          .0000
        17     1.6200+005                 .0000          .0000
        18     1.6200+005                 .0000          .0000
        19     2.5200+006                 .0000          .0000
        20     4.8000-001                 .0000          .0000
        21     4.8000-001                 .0000          .0000
        22     3.6000+004                 .0000          .0000
        23     3.6000+004                 .0000          .0000
        24     7.2000+005                 .0000          .0000
        25     1.4400-001                 .0000          .0000
```

Exhibit IX-9. Sample CPREP Output for the CHEMPARAM File

```
       26      2.2800+005                        .0000          .0000
       27      7.2000+005                        .0000          .0000
       28      7.2000+005                        .0000          .0000
       29      2.3000+005                        .0000          .0000
       30      4.6000+005                        .0000          .0000
       31      3.0000+004                        .0000          .0000
       32      3.0000+002                        .0000          .0000
       33      1.2000+004                        .0000          .0000
       34      3.0000+002                        .0000          .0000
       35      1.1400+006                        .0000          .0000
       36      8.1000-002  P                     .0000          .0000
       37      1.2150-001  P                     .0000          .0000
       38      6.0000+006                        .0000          .0000
       39      1.2000+005                        .0000          .0000
       40      1.6800+000                   1.2500+004     2.9800+002
       41      2.4000+005                        .0000          .0000
       42      2.4000+005                        .0000          .0000
       43      7.2000+005                        .0000          .0000
       44      4.8000+005                        .0000          .0000
       45      1.2000+005                        .0000          .0000
       46      7.2000+005                        .0000          .0000
       47      4.8000+005                        .0000          .0000
       48      1.2000+005                        .0000          .0000
       49      4.0200+004                        .0000          .0000
       50      1.4400+004                        .0000          .0000
       51      5.4000+003                        .0000          .0000
       52      9.0000+003                        .0000          .0000
       53      2.0400+004                        .0000          .0000
       54      2.5500+004                        .0000          .0000
       55      5.1000+003                        .0000          .0000
       56      3.6000+005                        .0000          .0000
       57      9.6000+004                        .0000          .0000
       58      9.0000+005                        .0000          .0000
       59      6.0000+006                        .0000          .0000
       60      1.8000+003                        .0000          .0000
       61      9.0000+002                        .0000          .0000
       62      2.1000+006                        .0000          .0000
       63      3.6000+001                        .0000          .0000
       64      6.0000+005                        .0000          .0000
       65      2.1600+000  P                     .0000          .0000
       66      5.4000+004                        .0000          .0000
       67      4.8000+004                        .0000          .0000
       68      5.4000+005                        .0000          .0000
       69      3.0000-002                        .0000          .0000
END
COEFFICIEN
ALFHA          5.00000-001
BETA           4.80000-001
GAMMA          1.00000+000
ETA            1.00000-001
END
```

Exhibit IX-9 (Continued)

```
****************  CHEMPARAM FILE  ******************

FILE DESCRIPTION HEADER RECORD
    FILE TYPE       = CHEMPARAM
    FILE ID         =   CHEMISTRY PARAMETERS  NEW CHEM  HIGHER PARAFINS LOWER LIMI
    NO OF SEGMENTS =  0
    NO OF SPECIES  = 11
    BEG DATE        =  0
    BEG TIME        = 0.
    END DATE        =  0
    END TIME        = 0.

SPECIES DESCRIPTION HEADER RECORD
    NO
    NO2
    O3
    ETH
    OLE
    PAR
    CARB
    ARO
    BZA
    PAN
    CO

CHEMISTRY DEFINITION RECORD
    MECHANISM ID     = CARBON BOND MECHANISM -- NOVEMBER 78
    NO OF REACTIONS = 69
    NO OF COEFFS     =  4

SPECIES PARAMETERS RECORD

    SPEC NAME   REACT   SSIC   SSBC       DVRES       LOW BD SS     UP BD SS     LOW BD NUM    UP BD NUM
    NO            T       F      F     2.8000-001    1.0000-005   1.0000+006   1.0000-005   1.0000+006
    NO2           T       F      F     1.1100-002    1.0000-004   1.0000+006   1.0000-004   1.0000+006
    O3            T       T      T     1.4700-002    1.0000-009   1.0000+006   1.0000-009   1.0000+006
    ETH           T       F      F     1.0000+010    1.0000-006   1.0000+006   1.0000-006   1.0000+006
    OLE           T       F      F     1.0000+010    1.0000-006   1.0000+006   1.0000-004   1.0000+006
    PAR           T       F      F     1.0000+010    1.0000-003   1.0000+006   1.0000-006   1.0000+006
    CARB          T       F      F     1.0000+010    1.0000-006   1.0000+006   1.0000-006   1.0000+006
    ARO           T       F      F     1.0000+010    1.0000-006   1.0000+006   1.0000-006   1.0000+006
    BZA           T       F      F     1.0000+010    1.0000-006   1.0000+006   1.0000-006   1.0000+006
    PAN           T       F      F     1.0000+010    1.0000-005   1.0000+006   1.0000-006   1.0000+006
    CO            T       F      F     1.0000+010    1.0000-002   1.0000+006   1.0000-002   1.0000+006

REACTION PARAMETERS RECORD

       RATE CONST  PHOTOL    TEMP     ACT ENERGY     REF TEMP
  1    6.0000+001     T        F        .0000          .0000
  2    2.6400+008     F        F        .0000          .0000
  3    1.4340+003     F        T     1.4500+003     2.9800+002
  4    2.8800+000     F        T     2.4500+003     2.9800+002
  5    8.0400+005     F        F        .0000          .0000
  6    4.6200+003     F        T     1.0000+003     2.9800+002
  7    3.0000+002     F        T     1.5250+003     2.9800+002
  8    8.4000+005     F        F        .0000          .0000
  9    2.6400+004     F        F        .0000          .0000
```

Exhibit IX-9 (Continued)

```
10   9.0000-003    F    F      .0000         .0000
11   1.6800+006    F    F      .0000         .0000
12   9.0000-003    F    T   -1.0600+004    2.9800+002
13   7.2000+005    F    F      .0000         .0000
14   9.0000+005    F    F      .0000         .0000
15   1.2000+003    F    F      .0000         .0000
16   9.0000+004    F    F      .0000         .0000
17   1.6200+005    F    F      .0000         .0000
18   1.6200+005    F    F      .0000         .0000
19   2.5200+006    F    F      .0000         .0000
20   4.8000-001    F    F      .0000         .0000
21   4.8000-001    F    F      .0000         .0000
22   3.6000+004    F    F      .0000         .0000
23   3.6000+004    F    F      .0000         .0000
24   7.2000+005    F    F      .0000         .0000
25   1.4400-001    F    F      .0000         .0000
26   2.2800+005    F    F      .0000         .0000
27   7.2000+005    F    F      .0000         .0000
28   7.2000+005    F    F      .0000         .0000
29   2.3000+005    F    F      .0000         .0000
30   4.6000+005    F    F      .0000         .0000
31   3.0000+004    F    F      .0000         .0000
32   3.0000+002    F    F      .0000         .0000
33   1.2000+004    F    F      .0000         .0000
34   3.0000+002    F    F      .0000         .0000
35   1.1400+006    F    F      .0000         .0000
36   8.1000-002    T    F      .0000         .0000
37   1.2150-001    T    F      .0000         .0000
38   6.0000+006    F    F      .0000         .0000
39   1.2000+005    F    F      .0000         .0000
40   1.6800+000    F    T    1.2500+004    2.9800+002
41   2.4000+005    F    F      .0000         .0000
42   2.4000+005    F    F      .0000         .0000
43   7.2000+005    F    F      .0000         .0000
44   4.8000+005    F    F      .0000         .0000
45   1.2000+005    F    F      .0000         .0000
46   7.2000+005    F    F      .0000         .0000
47   4.8000+005    F    F      .0000         .0000
48   1.2000+005    F    F      .0000         .0000
49   4.0200+004    F    F      .0000         .0000
50   1.4400+004    F    F      .0000         .0000
51   5.4000+003    F    F      .0000         .0000
52   9.0000+003    F    F      .0000         .0000
53   2.0400+004    F    F      .0000         .0000
54   2.5500+004    F    F      .0000         .0000
55   5.1000+003    F    F      .0000         .0000
56   3.6000+005    F    F      .0000         .0000
57   9.6000+004    F    F      .0000         .0000
58   9.0000+005    F    F      .0000         .0000
59   6.0000+006    F    F      .0000         .0000
60   1.8000+003    F    F      .0000         .0000
```

Exhibit IX-9 (Continued)

```
61   9.0000+002      F      F      .0000        .0000
62   2.1000+006      F      F      .0000        .0000
63   3.6000+001      F      F      .0000        .0000
64   6.0000+005      F      F      .0000        .0000
65   2.1600+000      T      F      .0000        .0000
66   5.4000+004      F      F      .0000        .0000
67   4.8000+004      F      F      .0000        .0000
68   5.4000+005      F      F      .0000        .0000
69   3.0000-002      F      F      .0000        .0000

STOICHIOMETRIC COEFFICIENTS RECORD
    ALPHA      5.0000-001
    BETA       4.8000-001
    GAMMA      1.0000+000
    ETA        1.0000-001
```

Exhibit IX-9 (Concluded)

B. THE SIMULATION CONTROLS FILE

The Simulation Controls (SIMCONTROL) file, generally the last to be prepared, is the input file likely to be varied the most frequently. As previously mentioned, this file can routinely be prepared as a separate job step within each airshed simulation run.

Figure IX-2 is an information flow diagram for use in setting up the job control for a SIMCONTROL file creation run. The program that creates the SIMCONTROL file is called SPREP. It requires as input a CONTROL packet and a SIMULATION packet, which are described in detail in the next section. The printed output from SPREP consists of input numbers, error messages, if any, and the values written to the SIMCONTROL file (see Section B.3 of this chapter for sample input and output listings). The file itself is written to FORTRAN Unit 1, and the file format is given in Chapter IX of the Systems Manual.

1. CONTROL Packet Rules for the SIMCONTROL File

An abbreviated CONTROL packet is used to create the SIMCONTROL file. The packet names and identifies the type of file to be created, and it must be entered before any other packet. The contents of each card in the CONTROL packet are described in Table IX-5, and the format is shown in Exhibit IX-10.

2. SIMULATION Packet Rules for the SIMCONTROL File

The SIMULATION packet must follow the CONTROL packet in the input deck used to create the SIMCONTROL file. The contents of each card in the SIMULATION packet are described in Table IX-6 and the format is shown in Exhibit IX-11.

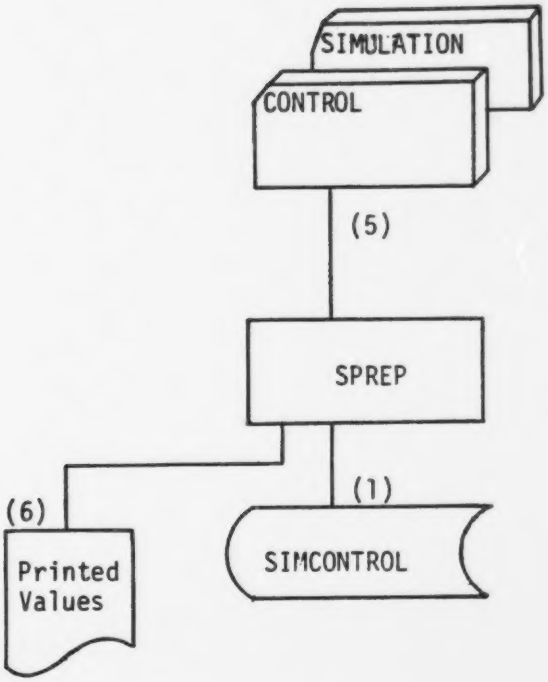

SIMULATION
CONTROL
(5)
SPREP
(6)
(1)
Printed Values
SIMCONTROL

Figure IX-2. Information Flow Diagram for Use in Creation of the SIMCONTROL File

Table IX-5. CONTROL Packet for the SIMCONTROL File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	10A1	--	Must be CONTROL, left adjusted
2 File Name	File name 1-10	10A1	--	Must be SIMCONTROL, left adjusted
3 File Identifier	Identifier 1-60	60A1	--	Any 60 characters; the file identifier will appear on the File Description Header Record
4 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number 1-10	11-20	21-30	31-40	41-50	51-60	FORTRAN Format
1	Packet Header	CONTROL						10A1
2	File Name	SIMCONTROL						10A1
3	File Identifier							60A1
4	Packet Terminator	END						10A1

Exhibit IX-10. CONTROL Packet Format for the SIMCONTROL File

Table IX-6. SIMULATION Packet for the SIMCONTROL File

Card Number and Name	Item and Columns	Format	Units	Comments
1 Packet Header	Header 1-10	10A1	--	Must be SIMULATION, left adjusted
2 File Identifier	Identifier 1-60	60A1	--	Any 60-characters; to provide a unique identifier, change this card for each run
3 Time Limits of the Run				Beginning date and time must appear within a time interval on the AIRQUALITY file, and the entire time span shown here must be included within the time span of every other time-varying data file; when restarting a run from an intermediate stopping point, these time limits must be changed
	Beginning date 1-10	I10	Julian date (yyddd)	yy is the last two digits of the year and ddd is the three-digit Julian date
	Beginning time 11-20	I10	Military time (hhmm)	hh is hours and mm is minutes--this time will be internally converted to hours and fraction
	End date 21-30	I10	Julian date (yyddd)	Same format as beginning date
	End time 31-40	I10	Military time (hhmm)	Same format as beginning time
4 Simulation Options				For each flag; .TRUE. means "yes, do it," and .FALSE. means "no, don't do it"
	Restart flag 1-10	L10	--	Set to TRUE if this is a restart; the simulation program will not perform steady-state computations on initial concentrations if the restart flag is TRUE

Table IX-6 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
4 (cont'd)	Surface removal flag 11-20	L10	--	Set to TRUE if the effects of pollutant uptake at the surface are to be calculated; when the surface removal flag is TRUE, there must be either a TERRAIN file or a nonzero vegetation factor specified on Card 6 of this packet
	PTSOURCE flag 21-30	L10	--	Set to TRUE if elevated point source emissions from a PTSOURCE file are to be included in the simulation; if flag is TRUE, there must be a PTSOURCE file; if it is FALSE, the PTSOURCE file, if present, will be ignored
	ROADWAY flag 31-40	L10	--	Set to TRUE if there is a ROADWAY file; flag may be reset to FALSE by the simulation program if there is no surface layer or if no reactive species are being simulated; if flag is TRUE, there must be a ROADWAY file; if flag is set to FALSE or reset to FALSE under the conditions described above, the ROADWAY file, if present, will be ignored. (Use FALSE).
	TEMPERATUR flag 41-50	L10	--	Set to TRUE if there is a TEMPERATUR file; if flag is TRUE, there must be a TEMPERATUR file; if it is FALSE, the TEMPERATUR file, if present, will be ignored; when flag is FALSE, an ambient temperature of 25°C will be assumed, and the nominal input values of the reaction rate constants will be employed in the chemistry calculations (i.e., temperature effects will be ignored)

Table IX-6 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
4 (cont'd)				
	TERRAIN flag 51-60	L10	--	Set to TRUE if there is a TERRAIN file; if flag is TRUE, the TERRAIN file must be included; if it is false, the TERRAIN file, if present, will be ignored; when flag is FALSE, a default value for surface roughness must be specified on Card 6 of this packet, and a default vegetation factor must also be specified on Card 6 if surface uptake effects are to be calculated
5 More Simulation Options	Concentration variation flag 1-10	L10	--	Set to TRUE if subgrid scale concentration variation is to be calculated; if flag is TRUE, concentration variation will be calculated at each time step and averaged over the same period that concentrations are averaged; the average concentration variations will be output on the VARIATION file; the flag will be reset to FALSE in the program if there is no surface layer or no ROADWAY file
6 Default Terrain Values				Must be included whether or not the values are required
	Default surface roughness 1-10	F10.0	m	This value will be used to calculate the vertical diffusivity if the TERRAIN file is not input to the run; if the TERRAIN file is input, this value will be ignored

Table IX-6 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
6 (cont'd)				
	Default vegetation factor 11-20	F10.0	--	Pollutant uptake capability of the surface relative to that of alfalfa; this value will be used to calculate surface deposition if the TERRAIN file is not input to the run; if the TERRAIN file is input or if surface removal effects are not to be calculated, this value will be ignored
7 Integration Controls	Maximum time slice 1-10	F10.0	hr	The largest simulation time interval during which the boundary conditions at the segment interfaces will be held constant; this parameter is used with the next one to determine the time slice size used in the Airshed Simulation Program (see Chapter IV); if the maximum slice is set very large (i.e., 1. or more), the calculated time slice will be limited by the maximum number of steps in a slice (or, if the time steps are very large, by the output time intervals or the intervals on the input files); if the maximum slice is set small relative to the typical time step calculated, it will be the limiting factor in computing the time slice size to be used
	Maximum number of steps in a slice 11-20	I10	--	This parameter is used with the previous one to calculate the time slice size used in the Airshed Simulation Program; if this number is set very large, the slice will be limited by the maximum time slice size; if the number is small, the slice will be limited by

Table IX-6 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
7 (cont'd)				the maximum number of the smallest time steps; if this number is set to 1, the boundary conditions at the segment interfaces will be updated at the end of every time step
8 Chemistry Integration Controls				
	• Minimum chemistry time step 1-10	F10.0	hr	Provides a lower limit on the chemistry step size; the overall time step size for each segment will be determined by the maximum wind speed in the segment; within each cell, however, the time step can be further reduced for the chemistry step; if the chemistry step fails to converge or gives negative concentrations at this step size, the program will terminate
	Maximum number of iterations 11-20	I10	--	If the chemistry step does not converge within this number of iterations for any cell at a given time step, the chemistry step size for that cell will be halved and the iterative procedure will begin again
	Relative error tolerance 21-30	F10.0	--	Convergence criterion for the chemistry step--when the relative change in concentration for all species is less than this number, the iterative procedure is said to have converged; if the relative change in concentration for any species is greater than this number, another iteration will be performed

Table IX-6 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
8 (cont'd)				
	Darkness criterion 31-40	F10.0	Same as for RADFACTOR on the METSCALARS file	If the calculated RADFACTOR, which varies continuously in time, is less than this number, night chemistry will be used; if the calculated RADFACTOR is greater than this number, the normal (daytime) chemistry will be used; if the simulation is performed on inert species only or if the night chemistry mechanism has been disabled, this number is ignored
9 Output Intervals	Instantaneous output interval 1-10	F10.0	hr	Instantaneous concentrations are written to the output file INSTANT at the beginning of the simulation and at this time interval thereafter; if the end of a time slice will go past the output time, the slice will be reduced to hit the output time exactly; instantaneous concentrations are also written when time-averaged concentrations are written, enabling a restart from the beginning of any averaging period
	Average output intervals 11-20	F10.0	hr	Starting at the beginning of the simulation, concentrations will be averaged over this interval and written to the AVERAGE file at the end of the interval; if the end of a time slice will go past the end of an averaging interval, the slice will be reduced to correspond to the end of the interval exactly

Table IX-6 (Continued)

Card Number and Name	Item and Columns	Format	Units	Comments
10 Print Options				Six options are read, but only five are used
	Print file history 1-10	I10	--	If this field is set to =1, a one-line message will be printed each time a time interval record is read on any data file; if set to blank or zero, the file read messages will not be printed
	Print storage allocation 11-20	I10	--	If this field is set to =1, all storage allocation pointers and controls will be printed; this information is useful only for program debugging; if set to blank or zero, the information will not be printed
	Print instantaneous concentrations 21-30	I10	--	If set positive, this is the number of vertical levels of concentrations that will be printed at the end of each instantaneous output interval (see Card 9); the boundary cells printed may contain irrelevant information and, therefore, the printouts should be used for debugging only; concentration maps will be printed for each segment, for each species, for each level up to the number specified, but not exceeding the number of levels modeled; if set to blank or zero, instantaneous concentrations will not be printed
	Print average concentrations 31-40	I10	--	If set positive, this is the number of vertical levels of average concentrations that will be printed at the end of each averaging interval (see Card 9); format and order of the average concentration printout is the same as that of the instantaneous concentration option; if set to blank or zero, average concentrations will not be printed

Table IX-6 (Concluded)

Card Number and Name	Item and Columns	Format	Units	Comments
10 (cont'd)				
	Print concentration variations 41-50	I10	--	If set positive, concentration variations will be printed after instantaneous and after average concentrations as selected above. If set to blank or zero, if both options above are zero, or if concentration variations are not calculated, concentration variations are not printed
11 Packet Terminator	Terminator 1-3	10A1	--	Must be END, left adjusted

Card Number	Card Identifier	Column Number						FORTRAN Format
		1-10	11-20	21-30	31-40	41-50	51-60	
1	Packet Header	SIMULATION						10A1
2	Run Identification							60A1
3	Time Limits of the Run	beg date	beg time	end date	end time			4I10
4	Simulation Options	restart	surface removal	pt srces	roadway	temp	terrain	6L10
5	More Simulation Options	conc vartn						6L10
6	Default Terrain Values	surface roughness	vegetation					2F10.0
7	Integration Time Interval Controls	max time slice	max # steps in slice					F10.0, I10
8	Chemistry Integration Controls	min chem step	max # iter	rel error tol	dark crit			F10.0, I10 2F10.0
9	Output intervals	instant	average					2F10.0
10	Print Options	file history	storage allocation	instant conc	average conc	conc vartn		6I10
11	Packet Terminator	END						10A1

Exhibit IX-11. SIMULATION Packet Format for the SIMCONTROL File

3. SPREP Sample Input and Output

Exhibit IX-12 is a listing of an input deck used to create a SIMCONTROL file. Exhibit IX-13 is the printout that was generated by SPREP; it first lists the values on the input cards as they are read in, and then shows these values put out to the SIMCONTROL file.

```
CONTROL
SIMCONTROL
RAPS TEST RUN CONTROLS FOR JUNE-JULY 1978
END
SIMULATION
RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79
     76195      0500     76195      0900
         F         T         T         F         T         T
         F
        .5        1.
        .1         1
      .003        20       .01       .01
        1.        1.
         1         1         1         1
END
```

Exhibit IX-12. Sample SPREP Input for the SIMCONTROL File

```
CONTROL
SIMCONTROL
RAPS TEST RUN CONTROLS FOR JUNE-JULY 1978
END
SIMULATION
RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79
     76195       500     76195       900
         F         T         T         F         T         T
         F
     5.0000-001     1.0000+000
     1.0000-001         1
     3.0000-003        20     1.0000-002     1.0000-002
     1.0000+000     1.0000+000
         1         1         1         1         0         0
END
```

Exhibit IX-13. Sample SPREP Output for the SIMCONTROL File

```
************** SIMCONTROL FILE ***********************

FILE DESCRIPTION HEADER RECORD
    FILE TYPE      = SIMCONTROL
    FILE ID        = RAPS TEST RUN CONTROLS FOR JUNE-JULY 1978
    NO OF SEGMENTS =  0
    NO OF SPECIES  =  0
    BEG DATE       =  0
    BEG TIME       = 0.
    END DATE       =  0
    END TIME       = 0.

SIMULATION CONTROLS RECORD
    RUN ID         = RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79

    BEG DATE       =      76195
    BEG TIME       =       5.00
    END DATE       =      76195
    END TIME       =       9.00

    RESTART FLAG   =          F
    SINK FLAG      =          T
    PTS  FLAG      =          T
    RWY  FLAG      =          F
    TEMP FLAG      =          T
    TERR FLAG      =          T

    CONC VAR FLAG  =          F

    DEF ROUGHNESS  =      .5000
    DEF VEGETAT'N  =     1.0000

    MAX TIME SLICE=       .1000
    MAX STEPS      =          1

    MIN STEP SIZE  =      .0030
    MAX ITERS      =         20
    ERR TOL        =    .010000
    DARK CRITERION=       .0100

    INST INTERVAL  =       1.00
    AVG  INTERVAL  =       1.00

    PRINT OPTIONS  =          1
                              1
                              1
                              1
                              0
                              0

@BRKPT PRINT$
```

Exhibit IX-13 (Concluded)

X AIRSHED SIMULATION

After all the input data files have been prepared as described in the preceding chapters, running the Airshed Simulation Program is simply a matter of properly assigning all the input files and arranging to save all the desired output files. That is, running the simulation is primarily a job control function, since the bulk of the input and output processing is performed outside of this step.

This chapter discusses job control in terms of input, scratch, and output files; describes and presents samples of the printed output; and discusses the error messages generated by the program. Also included is a worksheet that can be used to keep track of files.

A. JOB CONTROL

Figure X-1 shows the information flow for the Airshed Simulation Program. (Each group of files is discussed in more detail later.) Dotted lines indicate a possible creation of the SIMCONTROL file in a separate job step, and a possible restart using a previously generated output INSTANT file as an input AIRQUALITY file. Because the actual job control statements required are highly dependent on a particular implementation or computer, they are not specified here, but should be developed by the computer personnel who implement the system.

Tables X-1, X-2, and X-3 show the FORTRAN unit assignments of the Airshed Simulation Program's input, scratch, and output files, respectively. Currently, these unit assignments are compiled in the program by data statements in the subprogram BLKDAT. For instructions on changing the assignments, see Section VII.H. of the Systems Manual. The local file designation that corresponds to each data file should be entered in the tables for each specific implementation:

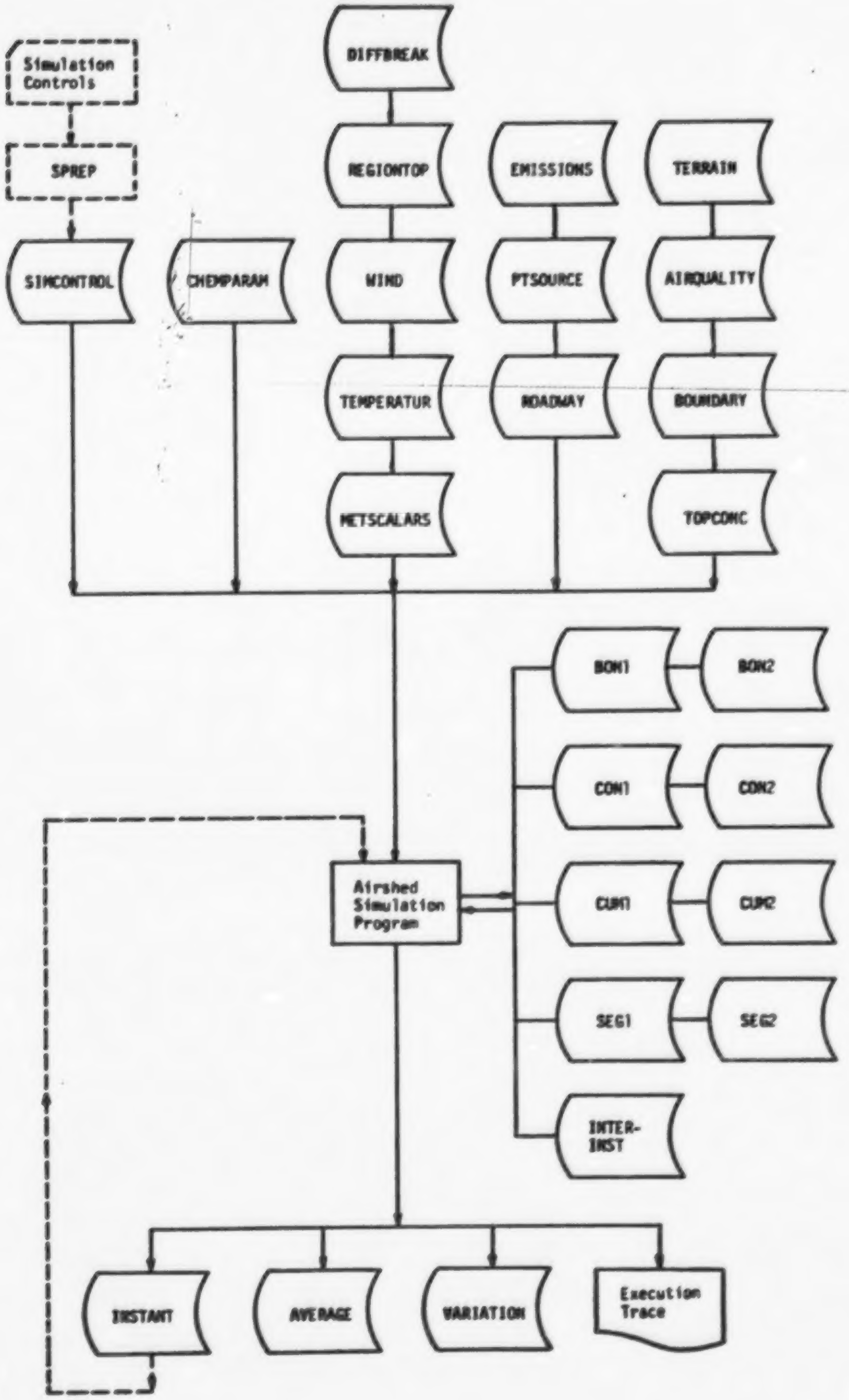

Simulation Controls
SPREP
DIFFBREAK
REGIONTOP
EMISSIONS
TERRAIN
SIMCONTROL
CHEMPARAM
WIND
PTSOURCE
AIRQUALITY
TEMPERATUR
ROADWAY
BOUNDARY
METSCALARS
TOPCONC
BON1
BON2
CON1
CON2
Airshed Simulation Program
CUM1
CUM2
SEG1
SEG2
INTER-INST
INSTANT
AVERAGE
VARIATION
Execution Trace

Figure X-1. Information Flow Diagram for the Airshed Simulation Program

Table X-1. Input File Assignments

File Name	Unit No.	LBL lfn*	Optional File	File Closed During Simulation
AIRQUALITY	3	AIRQ		✓
BOUNDARY	11	BOUND		
DIFFBREAK	12	DIFBK		
EMISSIONS	13	EMISS		
METSCALARS	7	METS		
PTSOURCE	14	POINTS	✓	
REGIONTOP	15	REGTOP		
ROADWAY	16	ROAD	✓	
TEMPERATUR	17	TEMP	✓	
TERRAIN	4	TERAIN	✓	✓
TOPCONC	18	TOPCON		
WIND	19	WIND		
CHEMPARAM	2	CPARAM		✓
SIMCONTROL	1	SIMCTL		✓

---

* "lfn" means local file name.

Table X-2. Scratch File Assignments

File Name	Unit No.	LBL lfn	Optional File	File Closed During Simulation
INTERINST	30	TAPE30		
BON1	37	†	*	
BON2	38	†	*	
CON1	33	TAPE33	*	
CON2	34	TAPE34		
CUM1	35	TAPE35	*	
CUM2	36	TAPE36		
SEG1	31	TAPE31	*	
SEG2	32	TAPE32		

---

* Not used for runs with only one segment.

† The LBL system utilizes large core memory instead of these files; UNIVAC uses extended memory.

Table X-3. Output File Assignments

File Name	Unit No.	LBL lfn	Optional File	File Closed During Simulation
AVERAGE	21	AVERAG	✓	
INSTANT	22	INST	✓	
VARIATION	23	CONVAR	✓	
Execution Trace	6	OUTPUT		

- > For the LBL CDC 7600 system, six-character mnemonic names are used instead of "TAPEnn."
- > For the UNIVAC 1100 systems, the internal file names are the unit numbers themselves.
- > For IBM systems, the DD names are of the form "FTnnF001."

1. Input Files

Table X-1 lists fourteen input files--twelve M.E.B. files and two control files. Four of the M.E.B. files are optional: PTSOURCE, ROADWAY, TEMPERATUR, and TERRAIN; all other input files must be present. For more information on selecting input file options and providing default values for the data omitted, see the Section IX.B on preparation of the SIMCONTROL file.

2. Scratch Files

Table X-2 shows the nine scratch files that might be used by the simulation. The actual number of files used and the method of assigning them are governed by the particular implementation of the system. For example, at LBL, only seven of the files are used, and the other two are represented by vectors in large core memory. See Section VII.B of the Systems Manual for more detailed information on the scratch files.

3. Output Files

As shown in Table X-3, the Airshed Simulation Program can write up to three binary data files, which are described in detail in Chapter IX of the Systems Manual. The presence or absence of these files is determined by parameters on the SIMCONTROL file:

> AVERAGE will be written if the averaging interval is less than 99.0 hours.
> INSTANT will be written at the beginning of the simulation, at the instantaneous output interval, and also at the end of each averaging interval if that time does not coincide with an instantaneous output time. If both the instantaneous output interval and the averaging interval are greater than 99.0 hours, INSTANT will not be written at all.
> VARIATION will be written if the concentration variation option is TRUE and the averaging interval is less than 99.0 hours.

B. PRINTED OUTPUT

The printed output from the simulation program appears on the Execution Trace file--ordinarily the standard print unit--and always contains at least the following information:

> A complete display of the contents of the SIMCONTROL and CHEMPARAM files.
> The region description as specified on the BOUNDARY file. This description serves as the standard for the run: the horizontal grid parameters on all other spatially varying files and the vertical distribution parameters on all other vertically varying files must match those of the BOUNDARY file.
> The header information from each M.E.B. file. If the files were uniquely identified at the times they were created, this information completely defines all data input to the run.
> A message when each non-time-varying file is closed.
> A message at the end of each time slice indicating elapsed CPU time (if the host computer provides the capability).
> A message at the termination of the run.

As indicated on the SIMCONTROL file, additional printed output options are also available that are primarily useful for debugging:

> The file history printout consists of a message printed whenever a time interval record is read from any file. During early simulation runs, this information can help the user follow the progress of the run.
> The storage allocation printout consists of tables listing pointers to scratch storage. Each entry is the relative location of a data array in a single storage vector. To interpret these tables, see Section VII.B of the Systems Manual.
> Instantaneous and average concentration arrays may be printed at the same time they are written on the files. They are printed by segments, within each segment by species, and within each species by vertical level. These printouts contain values in the boundary cells that do not necessarily represent the actual boundary values at the time; thus, they should be used only for program debugging or for preliminary runs for which the binary output files are not to be saved.

Exhibit X-1 is an annotated excerpt of the output from a successful Airshed Simulation Program run that contains samples of all the normal and optional information printed.

If the Airshed Simulation Program is unable to perform the chemistry step successfully for any cell, it will give a "crash printout," showing the values in all data arrays in the vicinity of the cell where the error occurred. Also included are the values in the local vectors used by the simulation. A sample of the crash printout is shown in Exhibit X-2. The user should examine this printout and look for anomalous values of

```
************** SIMCONTROL FILE **********************

FILE DESCRIPTION HEADER RECORD
    FILE TYPE      = SIMCONTROL
    FILE ID        = RAPS TEST RUN CONTROLS FOR JUNE-JULY 1978
    NO OF SEGMENTS =  0
    NO OF SPECIES  =  0
    BEG DATE       =  0
    BEG TIME       = 0.
    END DATE       =  0
    END TIME       = 0.

SIMULATION CONTROLS RECORD
    RUN ID         = RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79
    BEG DATE       =       76195
    BEG TIME       =        5.00
    END DATE       =       76195
    END TIME       =        9.00

    RESTART FLAG  =            F
    SINK FLAG     =            T
    PTS  FLAG     =            T
    RWY  FLAG     =            F
    TEMP FLAG     =            T
    TERR FLAG     =            T

    CONC VAR FLAG =            F

    DEF ROUGHNESS =       .5000
    DEF VEGETAT'N =      1.0000

    MAX TIME SLICE=       .1000
    MAX STEPS     =           1

    MIN STEP SIZE =       .0030
    MAX ITERS     =          20
    ERROR TOL     =     .010000
    DARK CRITERION=       .0100

    INST INTERVAL =        1.00
    AVG  INTERVAL =        1.00

    FILE HISTORY  =           1
    STORAGE ALLOC =           1
    LFVELS INST   =           1
    LEVELS AVG    =           1
    CONC VAR      =           0
    OPT 3         =           0

FILE  1  SIMCONTROL CLOSED.
```

Exhibit X-1. Annotated Excerpt of Output from an Airshed Simulation Program Run

```
***************  CHEMPARAM FILE  ******************

FILE DESCRIPTION HEADER RECORD
    FILE TYPE       = CHEMFAPAM
    FILE ID         =   CHEMISTRY PARAMETERS  NEW CHEM  HIGHER PARAFINS LOWER LIMI
    NO OF SEGMENTS =  0
    NO OF SPECIES  = 11
    BEG DATE        =  0
    BEG TIME        = 0.
    END DATE        =  0
    END TIME        = 0.

SPECIES DESCRIPTION HEADER RECORD
    NO
    NO2
    O3
    ETH
    OLE
    PAR
    CARB
    ARO
    BZA
    PAN
    CO

CHEMISTRY DEFINITION RECORD
    MECHANISM ID     = CARBON BOND MECHANISM -- NOVEMBER 78
    NO OF REACTIONS = 69
    NO OF COEFFS     =  4

SPECIES PARAMETERS RECORD

    SPEC NAME   REACT   SSIC   SSBC       DVRES      LOW BD SS      UP BD SS     LOW BD NUM      UP BD NUM
    NO              T      F      F   2.8000-001    1.0000-005    1.0000+006    1.0000-005    1.0000+006
    NO2             T      F      F   1.1100-002    1.0000-004    1.0000+006    1.0000-004    1.0000+006
    O3              T      T      T   1.4700-002    1.0000-009    1.0000+006    1.0000-009    1.0000+006
    ETH             T      F      F   1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
    OLE             T      F      F   1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
    PAR             T      F      F   1.0000+010    1.0000-003    1.0000+006    1.0000-004    1.0000+006
    CARB            T      F      F   1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
    ARO             T      F      F   1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
    BZA             T      F      F   1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
    PAN             T      F      F   1.0000+010    1.0000-006    1.0000+006    1.0000-006    1.0000+006
    CO              T      F      F   1.0000+010    1.0000-002    1.0000+006    1.0000-002    1.0000+006

REACTION PARAMETERS RECORD

        RATE CONST  PHOTOL    TEMP      ACT ENERGY      REF TEMP
   1    6.0000+001       T       F        .0000          .0000
   2    2.6400+008       F       F        .0000          .0000
   3    1.4340+003       F       T      1.4500+003     2.9800+002
   4    2.8000+000       F       T      2.4500+003     2.9800+002
   5    8.0400+005       F       F        .0000          .0000
   6    4.6200+003       F       T      1.0000+003     2.9800+002
   7    3.0000+002       F       T      1.5250+003     2.9800+002
   8    8.4000+005       F       F        .0000          .0000
   9    2.6400+004       F       F        .0000          .0000
```

Exhibit X-1 (Continued)

```
10    9.0000-003    F    F       .0000         .0000
11    1.6800+006    F    F       .0000         .0000
12    9.0000-003    F    T   -1.0600+004    2.9300+002
13    7.2000+005    F    F       .0000         .0000
14    9.0000+005    F    F       .0000         .0000
15    1.2000+003    F    F       .0000         .0000
16    9.0000+004    F    F       .0000         .0000
17    1.6200+005    F    F       .0000         .0000
18    1.6200+005    F    F       .0000         .0000
19    2.5200+006    F    F       .0000         .0000
20    4.8000-001    F    F       .0000         .0000
21    4.8000-001    F    F       .0000         .0000
22    3.6000+004    F    F       .0000         .0000
23    3.6000+004    F    F       .0000         .0000
24    7.2000+005    F    F       .0000         .0000
25    1.4400-001    F    F       .0000         .0000
26    2.2800+005    F    F       .0000         .0000
27    7.2000+005    F    F       .0000         .0000
28    7.2000+005    F    F       .0000         .0000
29    2.3000+005    F    F       .0000         .0000
30    4.6000+005    F    F       .0000         .0000
31    3.0000+004    F    F       .0000         .0000
32    3.0000+002    F    F       .0000         .0000
33    1.2000+004    F    F       .0000         .0000
34    3.0000+002    F    F       .0000         .0000
35    1.1400+006    F    F       .0000         .0000
36    8.1000-002    T    F       .0000         .0000
37    1.2150-001    T    F       .0000         .0000
38    6.0000+006    F    F       .0000         .0000
39    1.2000+005    F    F       .0000         .0000
40    1.6800+000    F    T    1.2500+004    2.9300+002
41    2.4000+005    F    F       .0000         .0000
42    2.4000+005    F    F       .0000         .0000
43    7.2000+005    F    F       .0000         .0000
44    4.8000+005    F    F       .0000         .0000
45    1.2000+005    F    F       .0000         .0000
46    7.2000+005    F    F       .0000         .0000
47    4.8000+005    F    F       .0000         .0000
48    1.2000+005    F    F       .0000         .0000
49    4.0200+004    F    F       .0000         .0000
50    1.4400+004    F    F       .0000         .0000
51    5.4000+003    F    F       .0000         .0000
52    9.0000+003    F    F       .0000         .0000
53    2.0400+004    F    F       .0000         .0000
54    2.5500+004    F    F       .0000         .0000
55    5.1000+003    F    F       .0000         .0000
56    3.6000+005    F    F       .0000         .0000
57    9.6000+004    F    F       .0000         .0000
58    9.0000+005    F    F       .0000         .0000
59    6.0000+006    F    F       .0000         .0000
60    1.0000+003    F    F       .0000         .0000
61    9.0000+002    F    F       .0000         .0000
```

Exhibit X-1 (Continued)

```
62     2.1000+006      F       F         .0000          .0000
63     3.6000+001      F       F         .0000          .0000
64     6.0000+005      F       F         .0000          .0000
65     2.1600+000      T       F         .0000          .0000
66     5.4000+004      F       F         .0000          .0000
67     4.8000+004      F       F         .0000          .0000
68     5.4000+005      F       F         .0000          .0000
69     3.0000-002      F       F         .0000          .0000

STOICHIOMETRIC COEFFICIENTS RECORD
    ALFHA        5.0000-001
    BETA         4.8000-001
    GAMMA        1.0000+000
    ETA          1.0000-001

 FILE  2  CHEMPARAM  CLOSED.
```

Exhibit X-1 (Continued)

```
LOCAL POINTERS

    1    1
    2    5
    3    9
    4   13
    5   17
    6   21
    7   25
    8   36
    9   47
   10  168
   11  185
   12  202
   13  219
   14  236
   15  253
   16  168
   17  172
   18  177
   19  188
   20  232
   21  237
   22  248
   23  253
   24  269
   25  285
   26  289
   27  253
   28  257
   29  261
   30  265
   31  269
   32  273
   33  278
   34  282
   35  253
   36  264
   37  275
   38  286
   39  407
   40  418
```

Exhibit X-1 (Continued)

```
BOUNDARY INDEX TABLE FOR SEGMENT  1

 ROW             WEST                   EAST
   1       0    0    0    0        0    0    0    0
   2       2    0    0    0       16    0    0    0
   3       2    0    0    0       16    0    0    0
   4       2    0    0    0       16    0    0    0
   5       2    0    0    0       16    0    0    0
   6       2    0    0    0       16    0    0    0
   7       2    0    0    0       16    0    0    0
   8       2    0    0    0       16    0    0    0
   9       2    0    0    0       16    0    0    0
  10       2    0    0    0       16    0    0    0
  11       2    0    0    0       16    0    0    0
  12       2    0    0    0       16    0    0    0
  13       2    0    0    0       16    0    0    0

 COL             SOUTH                  NORTH
   1       0    0    0    0        0    0    0    0
   2       2    0    0    0       11    2   36   53
   3       2    0    0    0       11    2   37   54
   4       2    0    0    0       11    2   38   55
   5       2    0    0    0       11    2   39   56
   6       2    0    0    0       11    2   40   57
   7       2    0    0    0       11    2   41   58
   8       2    0    0    0       11    2   42   59
   9       2    0    0    0       11    2   43   60
  10       2    0    0    0       11    2   44   61
  11       2    0    0    0       11    2   45   62
  12       2    0    0    0       11    2   46   63
  13       2    0    0    0       11    2   47   64
  14       2    0    0    0       11    2   48   65
  15       2    0    0    0       11    2   49   66
  16       2    0    0    0       11    2   50   67
  17       0    0    0    0        0    0    0    0
```

Exhibit X-1 (Continued)

```
BOUNDARY INDEX TABLE FOR SEGMENT  2

ROW            WEST                    EAST
  1       2    0    0    0      16    0    0    0
  2       2    0    0    0      16    0    0    0
  3       2    0    0    0      16    0    0    0
  4       2    0    0    0      16    0    0    0
  5       2    0    0    0      16    0    0    0
  6       2    0    0    0      16    0    0    0
  7       2    0    0    0      16    0    0    0
  8       2    0    0    0      16    0    0    0
  9       2    0    0    0      16    0    0    0
 10       2    0    0    0      16    0    0    0
 11       2    0    0    0      16    0    0    0
 12       2    0    0    0      16    0    0    0
 13       0    0    0    0       0    0    0    0

COL            SOUTH                   NORTH
  1       0    0    0    0       0    0    0    0
  2       3    1  172  155      12    0    0    0
  3       3    1  173  156      12    0    0    0
  4       3    1  174  157      12    0    0    0
  5       3    1  175  158      12    0    0    0
  6       3    1  176  159      12    0    0    0
  7       3    1  177  160      12    0    0    0
  8       3    1  178  161      12    0    0    0
  9       3    1  179  162      12    0    0    0
 10       3    1  180  163      12    0    0    0
 11       3    1  181  164      12    0    0    0
 12       3    1  182  165      12    0    0    0
 13       3    1  183  166      12    0    0    0
 14       3    1  184  167      12    0    0    0
 15       3    1  185  168      12    0    0    0
 16       3    1  186  169      12    0    0    0
 17       0    0    0    0       0    0    0    0
```

Exhibit X-1 (Continued)

```
RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79

***************  REGION DESCRIPTION  ***************


HORIZONTAL GRID                                  X          Y

     REFERENCE ORIGIN (UTM - METERS)        725000.    4252000.   (ZONE  15)

     REGION ORIGIN (M FROM REF. ORG.)       -19000.     -16000.

     CELL SPACING (M)                         4000.       4000.

     NUMBER OF CELLS                            17          22


VERTICAL DISTRIBUTION

     NO. CELLS IN LOWER LAYER =  2

     NO. CELLS IN UPPER LAYER =  2

     SURFACE LAYER HT (M)         =   0.

     MIN HT LOWER LAYER CELLS (M) =  50.

     MIN HT UPPER LAYER CELLS (M) = 200.

     TOTAL NO. VERTICAL CELLS =  4


SEGMENTS   IORGX  IORGY    NOX    NOY
     1         0      0     17     13
     2         0      9     17     13


BEGINNING OF TABLES RELATIVE TO BEGINNING OF AVAILABLE SPACE
  SEGMENT         1
  LOCAL         131
  BOUNDARY      559
  SEG SCRATCH  2295
  LAST WORD   22756
```

Exhibit X-1 (Continued)

```
SEGMENT ALLOCATION TABLE
            1       2
  1         0       0
  2         0       9
  3        17      17
  4        13      13
  5        80     129
  6         0       0
  7       221     221
  8       884     884
  9      9724    9724
 10      2431    2431
 11      1736    1736
 12         1    1737
 13      9724    9724
 14         0    9724
 15      9724    9724
 16         0    9724
 17     10101   10738
 18         0   10101
 19         0       0
 20         0       0
 21         0       0
 22         0       0
 23         0       0
 24         0       0
 25         0       0
 26         0       0
 27         0       0
 28         0       0
 29         1       1
 30         1       1
 31         1       1
 32         1       0
 33         0       1
 34         1       1
 35        53      53
 36       105     105
 37       173     173
 38         0       0
 39         0       0
 40         0     241
 41       241       0
 42         1       1
 43         1       1
 44       885     885
 45      2432    2432
```

Exhibit X-1 (Continued)

46	2653	2653
47	2874	2874
48	3095	3095
49	3316	3316
50	3537	3537
51	3758	3758
52	3979	3979
53	4200	4200
54	5084	5084
55	5968	5968
56	6189	6189
57	6410	6410
58	6631	6631
59	0	0
60	0	0
61	9062	9062
62	9142	9191
63	9222	9320
64	10102	10739
65	0	0

Exhibit X-1 (Continued)

```
RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79


----------------------------------------------------------

FILE - AIRQUALITY   ID =  INITIAL POLLUTANT CONCENTRATIONS  ST LOUIS  500  76195
   SEGMENTS =  2    SPECIES = 11
   TIME SPAN =  76195    5.00 TO  76195    5.02
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   4   2 2       .00      50.00     200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13

SPECIES ON AIRQUALITY FILE
 NO.  NAME          NO. WITHIN RUN
   1  NO             1
   2  NO2            2
   3  O3             3
   4  ETH            4
   5  OLE            5
   6  PAR            6
   7  CARB           7
   8  ARO            8
   9  BZA            9
  10  PAN           10
  11  CO            11
         FILSKP READS TIME INTERVAL  76195  5.00    76195  5.02    ON UNIT  3


----------------------------------------------------------

FILE = BOUNDARY     ID = BOUNDARY DEFINITION AND CONCENTRATIONS
   SEGMENTS =  2    SPECIES = 11
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   4   2 2       .00      50.00     200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13

SPECIES ON BOUNDARY   FILE
 NO.  NAME          NO. WITHIN RUN
   1  NO             1
   2  NO2            2
   3  O3             3
   4  ETH            4
   5  OLE            5
   6  PAR            6
   7  CARB           7
   8  ARO            8
   9  BZA            9
  10  PAN           10
  11  CO            11
         FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 11
```

Exhibit X-1 (Continued)

```
---------------------------------------------------------

FILE = DIFFBREAK    ID =    HEIGHT OF THE MIXED LAYER
   SEGMENTS =  2    SPECIES =  0
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   0   2 2       .00     50.00    200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13
          FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 12


---------------------------------------------------------

FILE = EMISSIONS    ID = RAPS EMISSIONS (17 X 22) DAY195  07/13/76
   SEGMENTS =  2    SPECIES =  8
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   0   2 2       .00     50.00    200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13

SPECIES ON EMISSIONS  FILE
 NO.  NAME        NO. WITHIN RUN
   1  NO           1
   2  NO2          2
   3  ETH          4
   4  OLE          5
   5  PAR          6
   6  CARB         7
   7  ARO          8
   8  CO          11
          FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 13


---------------------------------------------------------

FILE = METSCALARS   ID =     VALUES FOR METEOROLOGICAL SCALARS
   SEGMENTS =  0    SPECIES =  0
   TIME SPAN =  76195    4.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   4   2 2       .00     50.00    200.00
          FILSKP READS TIME INTERVAL  76195  4.00    76195  5.00    ON UNIT  7

    TGRADBELOW     TGRADABOVE     EXPCLASS       RADFACTOR      CONCWATER      ATMOSPRESS
        -.010           .004        -1.000            .008      12687.000            .990
          FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT  7


---------------------------------------------------------
```

Exhibit X-1 (Continued)

```
FILE = PTSOURCE     ID =    POINT SOURCES FOR ST. LOUIS  76195   4X4 GRID
   SEGMENTS =  2    SPECIES =  7
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   4   2 2       .00     50.00    200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13

SPECIES ON PTSOURCE   FILE
 NO.  NAME        NO. WITHIN RUN
   1  NO           1
   2  NO2          2
   3  OLE          5
   4  PAR          6
   5  CARB         7
   6  ARO          8
   7  CO          11
         FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 14


-----------------------------------------------------------

FILE = REGIONTOP    ID =    HEIGHT OF THE TOP OF THE MODELING REGION
   SEGMENTS =  2    SPECIES =  0
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   0   2 2       .00     50.00    200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13
         FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 15


-----------------------------------------------------------

FILE = TEMPERATUR   ID =    TEMPERATURE FIELD FOR ST. LOUIS  DAY 195
   SEGMENTS =  2    SPECIES =  0
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   0   2 2       .00     50.00    200.00

 SEGMENTS
        0         0        17        13
        0         9        17        13
         FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 17


-----------------------------------------------------------

FILE = TERRAIN      ID =    SURFACE ROUGHNESS AND VEGETATIVE FACTORS
   SEGMENTS =  2    SPECIES =  0
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   0   2 2       .00     50.00    200.00
```

Exhibit X-1 (Continued)

```
 SEGMENTS
        0        0        17        13
        0        9        17        13


-----------------------------------------------------------

FILE = TOPCONC      ID =    POLLUTANT CONCENTRATIONS ABOVE THE MODELING REGION
   SEGMENTS =  2    SPECIES = 11
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   0   2 2      .00     50.00    200.00

 SEGMENTS
        0        0        17        13
        0        9        17        13

SPECIES ON TOPCONC     FILE
 NO.  NAME          NO. WITHIN RUN
   1  NO             1
   2  NO2            2
   3  O3             3
   4  ETH            4
   5  OLE            5
   6  PAR            6
   7  CARB           7
   8  ARO            8
   9  BZA            9
  10  PAN           10
  11  CO            11
         FILSKP READS TIME INTERVAL  76195   .00    76195 24.00    ON UNIT 18


-----------------------------------------------------------

FILE = WIND         ID =    WIND FIELD FOR ST. LOUIS   DIVERGENCE     ALGORITHM USED
   SEGMENTS =  2    SPECIES =  0
   TIME SPAN =  76195    5.00 TO  76195   24.00
 725000.4252000.    15 -19000. -16000.     4000.   4000.    17  22   4   2 2      .00     50.00    200.00

 SEGMENTS
        0        0        17        13
        0        9        17        13
         FILSKP READS TIME INTERVAL  76195  5.00    76195  6.00    ON UNIT 19


-----------------------------------------------

    TGRADBELOW     TGRADABOVE     EXPCLASS       RADFACTOR      CONCWATER      ATMOSPRESS
       -.010           .004           .000           .084       12687.000           .990

  FILE  4  TERRAIN    CLOSED.
         TZERO  READS TIME INTERVAL  76195  6.00    76195  7.00    ON UNIT 12 DIFFBREAK
         TZERO  READS TIME INTERVAL  76195  6.00    76195  7.00    ON UNIT 15 REGIONTOP
```

Exhibit X-1 (Continued)

```
FILE  3  AIRQUALITY CLOSED.

   76195  5.00  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.089     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.09  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.178     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.18  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.267     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.27  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.356     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.36  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.445     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.45  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.534     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.53  SEG     WXMAX      WYMAX  DTMAX     DT NDT
                  1     22453.     9603.   .089   .089   1
                  2     22453.     9603.   .089   .089   1

TIME =  76195    5.624     SLICE =  .0891     ELAPSED CPU TIME =     .000 SECS     TOTAL ELAPSED CPU TIME =     .000 SECS

   76195  5.62  SEG     WXMAX      WYMAX  DTMAX     DT NDT
```

Exhibit X-1 (Continued)

```
               1    22453.     9603.   .089    .089    1
               2    22453.     9603.   .089    .089    1

TIME =  76195    5.713    SLICE =  .0891    ELAPSED CPU TIME =    .000 SECS    TOTAL ELAPSED CPU TIME =     .000 SECS

     76195  5.71  SEG      WXMAX      WYMAX  DTMAX      DT NDT
                    1    22453.     9603.   .089    .089    1
                    2    22453.     9603.   .089    .089    1

TIME =  76195    5.802    SLICE =  .0891    ELAPSED CPU TIME =    .000 SECS    TOTAL ELAPSED CPU TIME =     .000 SECS

     76195  5.80  SEG      WXMAX      WYMAX  DTMAX      DT NDT
                    1    22453.     9603.   .089    .089    1
                    2    22453.     9603.   .089    .089    1

TIME =  76195    5.891    SLICE =  .0891    ELAPSED CPU TIME =    .000 SECS    TOTAL ELAPSED CPU TIME =     .000 SECS

     76195  5.89  SEG      WXMAX      WYMAX  DTMAX      DT NDT
                    1    22453.     9603.   .089    .089    1
                    2    22453.     9603.   .089    .089    1

TIME =  76195    5.980    SLICE =  .0891    ELAPSED CPU TIME =    .000 SECS    TOTAL ELAPSED CPU TIME =     .000 SECS

     76195  5.98  SEG      WXMAX      WYMAX  DTMAX      DT NDT
                    1    22453.     9603.   .089    .020    1
                    2    22453.     9603.   .089    .020    1

TIME =  76195    6.000    SLICE =  .0202    ELAFSED CPU TIME =    .000 SECS    TOTAL ELAPSED CPU TIME =     .000 SECS
```

Exhibit X-1 (Continued)

```
RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79

AVG  CONCENTRATIONS AT 76195   6.00 FOR SPECIES  1 NO           SEGMENT= 1  LEVEL=1

            1          2          3          4          5          6          7          8          9         10         11         12
           13         14         15         16         17
 13  8.44-004   5.04-003   3.31-003   4.85-003   4.08-003   2.75-003   3.18-003   3.95-003   4.13-003   1.87-003   1.28-003   4.01-004
     4.22-004   5.02-004   4.38-004   3.56-004   3.19-004
 12  8.45-004   1.48-002   5.33-003   5.07-003   5.01-003   3.73-003   5.43-003   6.32-003   5.77-003   3.48-003   7.91-004   6.04-004
     5.06-004   4.47-004   2.98-004   2.74-004   3.20-004
 11  8.47-004   5.29-003   9.43-003   8.66-003   5.13-003   4.94-003   7.93-003   1.18-002   1.24-002   3.61-003   1.33-003   5.41-004
     4.66-004   3.19-004   3.77-004   3.18-004   3.20-004
 10  8.48-004   2.38-003   4.72-003   4.76-003   4.03-003   3.34-003   3.62-003   2.89-003   2.21-003   1.78-003   1.35-003   4.64-004
     5.56-004   4.52-004   5.52-004   5.00-004   3.21-004
  9  8.50-004   1.45-003   2.57-003   4.12-003   4.34-003   2.72-003   2.48-003   2.56-003   2.23-003   4.71-004   4.17-004   4.99-004
     6.03-004   7.12-004   6.07-004   4.27-004   3.22-004
  8  8.51-004   1.12-003   1.48-003   1.99-003   2.94-003   3.52-003   3.25-003   1.15-003   5.71-004   4.51-004   2.87-004   3.09-004
     4.08-004   6.75-004   7.37-004   4.88-004   3.22-004
  7  8.53-004   8.15-004   8.88-004   1.05-003   1.31-003   1.81-003   1.44-003   1.23-003   4.94-004   4.00-004   2.79-004   2.87-004
     3.02-004   3.71-004   4.63-004   5.07-004   3.23-004
  6  8.54-004   4.91-004   6.41-004   8.83-004   1.14-003   1.46-003   5.81-004   5.00-004   4.34-004   4.55-004   3.41-004   2.93-004
     3.05-004   3.64-004   4.10-004   4.14-004   3.23-004
  5  8.56-004   4.07-004   5.30-004   7.01-004   8.49-004   1.52-003   5.45-004   4.00-004   3.29-004   2.98-004   3.13-004   2.72-004
     3.08-004   3.55-004   3.94-004   4.17-004   3.24-004
  4  8.57-004   3.25-004   4.37-004   5.52-004   8.59-004   1.59-003   4.73-004   3.34-004   3.07-004   2.96-004   3.33-004   2.56-004
     2.91-004   3.36-004   3.75-004   3.85-004   3.25-004
  3  8.59-004   2.62-004   3.38-004   4.93-004   1.18-003   4.14-003   2.68-004   2.89-004   3.01-004   3.05-004   3.60-004   2.55-004
     2.71-004   3.09-004   3.40-004   3.40-004   3.25-004
  2  3.01-004   2.56-004   3.07-004   3.43-004   5.22-004   7.81-004   2.69-004   2.95-004   2.95-004   2.88-004   2.78-004   2.75-004
     2.67-004   2.77-004   2.95-004   3.12-004   3.26-004
  1  2.00-003   3.03-004   3.05-004   3.06-004   3.08-004   3.09-004   3.11-004   3.12-004   3.14-004   3.15-004   3.17-004   3.18-004
     3.20-004   3.22-004   3.23-004   3.25-004   2.00-003

AVG  CONCENTRATIONS AT 76195   6.00 FOR SPECIES  2 NO2          SEGMENT= 1  LEVEL=1

            1          2          3          4          5          6          7          8          9         10         11         12
           13         14         15         16         17
 13  9.16-003   1.76-002   1.89-002   2.41-002   2.45-002   2.07-002   2.07-002   2.13-002   2.05-002   1.52-002   1.25-002   7.28-003
     6.64-003   6.24-003   5.03-003   4.01-003   3.68-003
 12  9.15-003   2.27-002   2.03-002   2.24-002   2.34-002   2.14-002   2.36-002   2.48-002   2.48-002   2.17-002   1.06-002   8.43-003
     6.68-003   5.65-003   4.26-003   3.67-003   3.68-003
 11  9.15-003   1.69-002   2.26-002   2.40-002   2.17-002   2.17-002   2.51-002   2.90-002   3.09-002   2.49-002   1.29-002   7.44-003
     5.95-003   4.84-003   4.75-003   3.89-003   3.68-003
 10  9.15-003   1.29-002   1.83-002   1.99-002   1.99-002   1.94-002   2.07-002   2.04-002   1.85-002   1.57-002   1.13-002   6.95-003
     6.87-003   5.82-003   5.71-003   4.63-003   3.68-003
  9  9.15-003   9.62-003   1.34-002   1.72-002   1.87-002   1.66-002   1.66-002   1.73-002   1.56-002   7.61-003   6.71-003   6.94-003
     7.30-003   7.43-003   5.89-003   4.29-003   3.68-003
  8  9.15-003   7.96-003   9.83-003   1.14-002   1.44-002   1.62-002   1.57-002   1.02-002   7.50-003   6.28-003   5.20-003   5.27-003
     5.85-003   6.96-003   6.49-003   4.61-003   3.68-003
  7  9.15-003   6.18-003   6.84-003   7.98-003   9.56-003   1.12-002   1.02-002   9.11-003   5.95-003   5.28-003   4.79-003   4.72-003
     4.66-003   4.88-003   4.87-003   4.59-003   3.68-003
  6  9.15-003   4.86-003   5.81-003   7.13-003   8.57-003   9.35-003   6.29-003   5.93-003   5.56-003   5.48-003   4.90-003   4.58-003
     4.54-003   4.89-003   4.27-003   4.17-003   3.68-003
  5  9.14-003   4.36-003   5.13-003   6.19-003   7.53-003   9.26-003   5.66-003   4.97-003   4.69-003   4.50-003   4.47-003   4.18-003
     4.26-003   4.35-003   4.30-003   4.14-003   3.68-003
```

Exhibit X-1 (Continued)

```
  4  9.14-003  3.90-003  4.54-003  5.48-003  7.47-003  9.28-003  4.80-003  4.43-003  4.35-003  4.30-003  4.36-003  3.91-003
     4.05-003  4.18-003  4.18-003  3.99-003  3.68-003
  3  9.14-003  3.55-003  4.05-003  5.30-003  8.91-003  1.40-002  3.55-003  4.04-003  4.16-003  4.20-003  4.31-003  3.75-003
     3.80-003  3.92-003  3.93-003  3.79-003  3.67-003
  2  3.70-003  3.52-003  3.79-003  4.15-003  5.16-003  5.81-003  3.63-003  3.87-003  3.90-003  3.86-003  3.80-003  3.69-003
     3.62-003  3.64-003  3.66-003  3.67-003  3.67-003
  1  2.00-003  3.70-003  3.70-003  3.69-003  3.69-003  3.69-003  3.69-003  3.69-003  3.69-003  3.68-003  3.68-003  3.68-003
     3.68-003  3.68-003  3.68-003  3.68-003  2.00-003

AVG  CONCENTRATIONS AT 76195   6.00 FOR SPECIES  3 03          SEGMENT= 1  LEVEL=1

            1         2         3         4         5
           13        14        15        16        17         6         7         8         9        10        11        12
 13  2.08-002  1.10-002  1.33-002  1.21-002  1.41-002  1.82-002  1.85-002  1.75-002  1.69-002  2.16-002  2.58-002  3.18-002
     3.16-002  3.07-002  2.98-002  2.50-002  2.43-002
 12  2.08-002  6.92-003  1.14-002  1.23-002  1.35-002  1.63-002  1.51-002  1.44-002  1.43-002  1.96-002  2.84-002  3.36-002
     3.29-002  3.15-002  2.93-002  2.52-002  2.43-002
 11  2.08-002  1.06-002  8.51-003  9.60-003  1.32-002  1.40-002  1.17-002  9.47-003  9.39-003  2.07-002  2.99-002  3.69-002
     3.62-002  3.41-002  3.02-002  2.62-002  2.43-002
 10  2.08-002  1.47-002  1.23-002  1.31-002  1.50-002  1.66-002  1.64-002  1.83-002  2.06-002  2.55-002  2.95-002  3.66-002
     3.48-002  3.35-002  2.91-002  2.54-002  2.43-002
  9  2.08-002  1.68-002  1.47-002  1.32-002  1.43-002  1.74-002  1.77-002  1.88-002  2.22-002  3.09-002  3.27-002  3.29-002
     3.22-002  3.10-002  2.83-002  2.54-002  2.43-002
  8  2.09-002  1.83-002  1.69-002  1.53-002  1.48-002  1.45-002  1.59-002  2.20-002  2.62-002  2.90-002  3.14-002  3.20-002
     3.12-002  2.92-002  2.74-002  2.53-002  2.43-002
  7  2.09-002  1.79-002  1.71-002  1.71-002  1.72-002  1.70-002  1.91-002  2.15-002  2.57-002  2.80-002  3.04-002  3.14-002
     3.09-002  2.90-002  2.55-002  2.39-002  2.43-002
  6  2.09-002  1.94-002  1.85-002  1.79-002  1.77-002  1.83-002  2.22-002  2.37-002  2.54-002  2.71-002  2.93-002  3.08-002
     3.06-002  2.94-002  2.31-002  2.35-002  2.43-002
  5  2.09-002  2.04-002  1.97-002  1.92-002  1.88-002  1.83-002  2.24-002  2.41-002  2.54-002  2.67-002  2.76-002  2.81-002
     2.73-002  2.57-002  2.41-002  2.33-002  2.43-002
  4  2.09-002  2.15-002  2.10-002  2.05-002  1.93-002  1.84-002  2.32-002  2.43-002  2.52-002  2.60-002  2.64-002  2.69-002
     2.65-002  2.56-002  2.43-002  2.33-002  2.43-002
  3  2.09-002  2.27-002  2.23-002  2.14-002  1.86-002  1.48-002  2.45-002  2.47-002  2.51-002  2.56-002  2.57-002  2.61-002
     2.59-002  2.52-002  2.41-002  2.33-002  2.43-002
  2  2.43-002  2.33-002  2.32-002  2.30-002  2.23-002  2.20-002  2.43-002  2.44-002  2.47-002  2.50-002  2.52-002  2.50-002
     2.49-002  2.45-002  2.39-002  2.33-002  2.43-002
  1  2.00-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002  2.43-002
     2.43-002  2.43-002  2.43-002  2.43-002  2.00-002

AVG  CONCENTRATIONS AT 76195   6.00 FOR SPECIES  4 ETH         SEGMENT= 1  LEVEL=1

            1         2         3         4         5
           13        14        15        16        17         6         7         8         9        10        11        12
 13  1.71-003  5.07-003  6.97-003  9.06-003  9.41-003  6.57-003  5.67-003  5.38-003  4.87-003  2.99-003  2.39-003  1.98-003
     1.94-003  1.96-003  1.64-003  1.10-003  1.09-003
 12  1.71-003  4.86-003  5.59-003  6.55-003  6.84-003  6.18-003  6.41-003  6.34-003  5.47-003  4.16-003  2.55-003  2.44-003
     2.15-003  1.94-003  1.41-003  1.06-003  1.09-003
 11  1.71-003  4.09-003  5.25-003  5.35-003  5.52-003  5.66-003  6.80-003  6.89-003  6.40-003  5.36-003  4.04-003  2.85-003
     2.25-003  1.72-003  1.53-003  1.18-003  1.09-003
 10  1.71-003  3.65-003  4.62-003  4.95-003  4.68-003  4.73-003  4.77-003  4.20-003  3.39-003  2.98-003  2.70-003  2.79-003
     2.71-003  2.20-003  2.07-003  1.57-003  1.09-003
  9  1.71-003  2.44-003  2.94-003  3.73-003  4.38-003  4.05-003  3.85-003  3.35-003  2.40-003  2.11-003  2.18-003  2.37-003
     2.56-003  2.62-003  2.09-003  1.33-003  1.09-003
  8  1.71-003  1.64-003  2.08-003  2.57-003  3.36-003  3.75-003  3.64-003  2.41-003  1.66-003  1.72-003  1.47-003  1.55-003
```

Exhibit X-1 (Continued)

```
      1.84-003  2.40-003  2.31-003  1.39-003  1.09-003
   7  1.71-003  1.49-003  1.77-003  1.93-003  2.27-003  2.53-003  2.16-003  1.78-003  1.61-003  1.61-003  1.32-003  1.35-003
      1.38-003  1.49-003  1.49-003  1.39-003  1.09-003
   6  1.71-003  1.37-003  1.50-003  1.84-003  2.11-003  2.14-003  1.47-003  1.33-003  1.47-003  1.77-003  1.42-003  1.28-003
      1.32-003  1.45-003  1.27-003  1.23-003  1.09-003
   5  1.71-003  1.38-003  1.42-003  1.51-003  1.61-003  1.99-003  1.28-003  1.13-003  1.19-003  1.26-003  1.27-003  1.17-003
      1.21-003  1.27-003  1.27-003  1.21-003  1.09-003
   4  1.71-003  1.28-003  1.38-003  1.45-003  1.66-003  2.08-003  1.28-003  1.11-003  1.15-003  1.21-003  1.29-003  1.13-003
      1.16-003  1.21-003  1.21-003  1.16-003  1.09-003
   3  1.71-003  1.14-003  1.22-003  1.32-003  1.63-003  2.17-003  1.07-003  1.13-003  1.16-003  1.22-003  1.33-003  1.14-003
      1.14-003  1.16-003  1.16-003  1.11-003  1.09-003
   2  1.09-003  1.12-003  1.18-003  1.20-003  1.31-003  1.40-003  1.09-003  1.13-003  1.13-003  1.14-003  1.14-003  1.13-003
      1.11-003  1.12-003  1.13-003  1.11-003  1.09-003
   1  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003  1.09-003
      1.09-003  1.09-003  1.09-003  1.09-003  1.09-003


 AVG  CONCENTRATIONS AT 76195   6.00 FOR SPECIES  5 OLE        SEGMENT= 1  LEVEL=1

             1         2         3         4         5         6         7         8         9        10        11        12
            13        14        15        16        17
  13  3.48-003  9.23-003  1.24-002  1.51-002  1.48-002  9.94-003  8.48-003  8.05-003  7.35-003  5.12-003  4.05-003  3.41-003
      3.25-003  3.15-003  2.75-003  2.16-003  2.20-003
  12  3.48-003  8.01-003  9.45-003  1.07-002  1.07-002  9.33-003  9.42-003  9.57-003  8.37-003  6.39-003  4.23-003  3.98-003
      3.51-003  3.16-003  2.53-003  2.12-003  2.20-003
  11  3.48-003  6.37-003  7.91-003  8.14-003  5.27-003  8.32-003  9.63-003  1.01-002  9.83-003  8.28-003  6.21-003  4.43-003
      3.63-003  2.96-003  2.66-003  2.27-003  2.20-003
  10  3.48-003  5.36-003  6.58-003  6.96-003  6.57-003  6.64-003  6.80-003  6.46-003  6.12-003  6.64-003  4.76-003  4.27-003
      4.05-003  3.42-003  3.20-003  2.65-003  2.20-003
   9  3.48-003  3.80-003  4.49-003  5.43-003  5.72-003  5.45-003  5.48-003  5.11-003  4.33-003  3.81-003  3.73-003  3.78-003
      3.84-003  3.80-003  3.21-003  2.42-003  2.20-003
   8  3.48-003  2.78-003  3.36-003  3.78-003  4.61-003  5.06-003  5.04-003  3.83-003  3.04-003  3.07-003  2.82-003  2.84-003
      3.06-003  3.55-003  3.41-003  2.48-003  2.20-003
   7  3.48-003  2.55-003  2.85-003  3.04-003  3.42-003  3.72-003  3.44-003  3.17-003  2.84-003  2.84-003  2.53-003  2.53-003
      2.53-003  2.62-003  2.58-003  2.48-003  2.20-003
   6  3.48-003  2.43-003  2.56-003  2.90-003  3.19-003  3.24-003  2.58-003  2.46-003  2.60-003  2.90-003  2.54-003  2.40-003
      2.43-003  2.66-003  2.33-003  2.31-003  2.20-003
   5  3.48-003  2.44-003  2.48-003  2.56-003  2.67-003  3.05-003  2.34-003  2.20-003  2.26-003  2.34-003  2.34-003  2.24-003
      2.27-003  2.34-003  2.34-003  2.30-003  2.20-003
   4  3.48-003  2.34-003  2.43-003  2.50-003  2.72-003  3.13-003  2.33-003  2.16-003  2.20-003  2.26-003  2.34-003  2.19-003
      2.21-003  2.27-003  2.28-003  2.24-003  2.20-003
   3  3.48-003  2.20-003  2.28-003  2.38-003  2.69-003  3.23-003  2.12-003  2.18-003  2.21-003  2.27-003  2.38-003  2.19-003
      2.19-003  2.22-003  2.22-003  2.20-003  2.20-003
   2  2.20-003  2.19-003  2.24-003  2.26-003  2.37-003  2.47-003  2.16-003  2.19-003  2.20-003  2.20-003  2.20-003  2.19-003
      2.18-003  2.19-003  2.20-003  2.20-003  2.20-003
   1  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003  2.20-003
      2.20-003  2.20-003  2.20-003  2.20-003  2.20-003
```

Exhibit X-1 (Concluded)

```
SUBROUTINE CRASH SHOWS YOU WHAT WAS WHAT AT THE TIME OF THE CRASH IN STEP 3, CELL   6,  4,  5, OF SEGMENT  1--SPECIES  1= CO


VALUES IN SPATIAL ARRAYS WILL BE PRINTED IN MAP FORM, I.E.
   N
 W   E
   S
WITH THE OFFENDING CELL ( 6, 4) IN THE CENTER


( 5, 5)  ( 6, 5)  ( 7, 5)
( 5, 4)  ( 6, 4)  ( 7, 4)
( 5, 3)  ( 6, 3)  ( 7, 3)


CONCENTRATIONS FOR SPECIES  1   CO

LEVELS             1                                       2                                       3
      1.293E+00  1.220E+00  1.000E-01    1.373E+00  1.231E+00  1.000E-01    1.263E+00  1.206E+00  1.000E-01
      1.218E+00  1.210E+00  1.000E-01    1.214E+00  1.216E+00  1.000E-01    1.200E+00  1.202E+00  1.000E-01
      1.195E+00  1.206E+00  1.000E-01    1.195E+00  1.205E+00  1.000E-01    1.188E+00  1.193E+00  1.000E-01

LEVELS             4                                       5
      1.202E+00  1.185E+00  1.000E-01    1.020E+00  1.019E+00  1.000E-01
      1.171E+00  1.183E+00  1.000E-01    9.535E-01  1.019E+00  1.000E-01
      1.165E+00  1.167E+00  1.000E-01    9.534E-01  9.528E-01  1.000E-01


  DIFFUSION BREAK                                          TOP OF REGION
        BEG                          END                         BEG                                  END
      52.      52.      52.       54.      54.      54.        189.0      189.0      189.0       198.1      198.1      198.1
      52.      52.      52.       54.      54.      54.        189.0      189.0      189.0       198.1      198.1      198.1
      52.      52.      52.       54.      54.      54.        189.0      189.0      189.0       198.1      198.1      198.1


       TEMP                    ROUGH               VEG                        CARM
  288.7  288.7  288.7      .5      .5      .5    1.00  1.00  1.00     1.00E-01  1.00E-01  1.00E-01
  288.7  288.7  288.7      .5      .5      .5    1.00  1.00  1.00     1.00E-01  1.00E-01  1.00E-01
  288.7  288.7  288.7      .5      .5      .5     .93  1.00  1.00     1.00E-01  1.00E-01  1.00E-01
```

Exhibit X-2. Sample Crash Output from the Airshed Simulation Program

```
LEVEL                 WX                                         WY
  1
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
  2
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
  3
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
  4
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
  5
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04
          3.000E+03   3.000E+03   3.000E+03     -1.000E+04  -1.000E+04  -1.000E+04

SPECIES             QT                                    QR                                          CTOP

 1=CO
      1.559E+01   5.772E+00   1.934E+00     1.000E-01   1.000E-01   1.000E-01     1.000E-01   1.000E-01   1.000E-01
      9.193E-01   2.197E+00   1.152E+00     1.000E-01   1.000E-01   1.000E-01     1.000E-01   1.000E-01   1.000E-01
      0.          1.027E+00   3.249E-01     1.000E-01   1.000E-01   1.000E-01     1.000E-01   1.000E-01   1.000E-01

BOUNDARY INDICES
 BDY    I     J          ADJ SEG    IJ WITHIN THAT SEGMENT
  W     2     4                0    0
  E     6     4                0    0
  S     6     2                0    0
  N     6    11                0    0

SPEC            2           3           4           5
  1     1.00E-01    1.00E-01    1.00E-01    1.00E-01
  1     1.00E-01    1.00E-01    1.00E-01    1.00E-01
  1     1.00E-01    1.00E-01    1.00E-01    1.00E-01
  1     1.00E-01    1.00E-01    1.00E-01    1.00E-01
```

Exhibit X-2 (Continued)

ut 5.2

Ck = -1

```
LOCAL VARIABLES

K   THOLD    THNEW    THAVG      HTOLD    HTNEW    HTAVG       AER   FACT        WZOLD         WZNEW          XKZ
1    20.      20.      20.        10.      10.      10.         0.   0.0000   0.            0.             0.
2    20.      20.      20.        30.      30.      30.         0.   0.0000   0.            0.             2.319E+03
3    20.      20.      20.        50.      50.      50.         0.   0.0000   0.            0.             2.432E+03
4    20.      20.      20.        70.      70.      70.         0.   0.0000   0.            0.             2.224E+03
5   109.     118.     114.       134.     139.     137.         0.   0.0000   0.            0.             1.954E+03
6                                                              0.   0.0000   -2.491E+02    -2.700E+02     7.835E+02


CONTEM ARRAY (STEPS 3 AND 4)
SPEC          1           2           3           4           5
  1      1.216E+00   1.217E+00   1.198E+00   1.169E+00   9.529E-01


SPEC        VD          SRC        FLUX
  1    1.000E-10   0.             2.197E+00


STEP 3 VECTORS

K       Y1-1        Y1-2        Y1-3          A           B           C           Y           X        CTEST        Z       AOMEGA



 1   0.          0.          0.          0.          0.          0.          0.          0.          1.22E+00   9.38E-01   1.30E+00
 2   0.          6.96E-01    3.04E-01    0.          1.30E+00    -3.04E-01   1.22E+00    1.22E+00    1.23E+00   9.83E-01   1.51E+00
 3   3.04E-01    4.18E-01    2.78E-01    -3.04E-01   1.58E+00    -2.78E-01   1.20E+00    1.20E+00    1.20E+00   1.12E+00   1.30E+00
 4   2.78E-01    6.46E-01    7.57E-02    -2.78E-01   1.35E+00    -7.07E-02   1.18E+00    1.17E+00    1.18E+00   9.53E-01   1.01E+00
 5   1.28E-02    9.10E-01    0.          -1.20E-02   1.01E+00    0.          9.50E-01    9.53E-01    1.02E+00   0.         0.

MET SCALARS

  TGRADBELOW   TGRADABOVE   EXPCLASS    RADFACTOR    CONCWATER    ATMOSPRESS
     -.009         .029      -1.000        .220     13000.000         .840

      ATFACT       TMBEG       TMEND       FRKBEG       FRKDEL        FACTRK
        .001       5.000       6.000        0.000         .220          .055
```

Exhibit X-2 (Continued)

```
MISC SCALARS

      ZREF        WXMAX        WYMAX         WAVW         WAVE         WAVS         WAVN
    10.000     3000.000    10000.000    10440.307    10440.307    10440.307    10440.307

     DTMAX           DT          NDT         ISEQ
      .322         .100            1            2

        EL        USTAR       DIFRES
    62.889      986.072         .014
TIME =  76210    5.300    SLICE =  .1000    ELAPSED CPU TIME =     .096 SECS    TOTAL ELAPSED CPU TIME =     3.736 SECS
```

Exhibit X-2 (Concluded)

any data. Check that printed values correspond to the data expected from the input files.

If no readily apparent errors can be found in the model inputs, then the available input and output should be examined by someone familiar with the technical components of the model. In undertaking the diagnosis, one should note the cause of the failure (iteration limit exceeded or negative concentration predicted). First, attention should be given to reaction rate constants and stoichiometric coefficients. Next, the predicted concentrations should be examined. Usually, one will note predictions for one or more pollutants that fall outside the expected nominal range of values for the particular contaminants in question. The development of an understanding of how these concentration values occurred will often suggest means for resolving the problem. For example, a very high NO concentration prediction may be causing the model to predict negative O_3 concentrations. The user might subsequently find that the NO emissions rate from a point source was in error by a factor of 100. Skill in diagnosing such problems requires some familiarity with the physical and chemical processes that take place in the atmosphere as well as an understanding of how these processes are treated in the model.

C. ERROR CONDITIONS

Table X-4 lists error conditions that could cause the Airshed Simulation Program to terminate before the simulation is completed. These are situations detected by the program itself rather than by the operating system, and the program will exit normally. Included in the table are the names of the subroutines in which the error messages are printed.

Table X-4. Airshed Simulation Program Error Conditions

Error Condition	Subroutine(s) That Print Errors
Control file errors	
File improperly named	SCREAD, CHREAD
Species or coefficient required by built-in chemical mechanism is missing	SPECID
Reactive species not listed in built-in mechanism	SPECID
Allocation errors	
Space allocation exceeded--region dimensions too large	ALLOC
M.E.B. file errors	
File missing or improperly named	HDRCK
Time span on file does not encompass time span of run	HDRCK
Region or segment definition does not match that on BOUNDARY file	HDRCK
Time intervals on file are not contiguous	FILSKP, FILCK
Unexpected end-of-file	Any file-read routine
Chemistry errors	
Negative concentrations at minimum step size	STEP4
Nonconvergence of concentration values at minimum step size	STEP4
Nonconvergence of $[HO_2]$ iteration	CHEM
Other errors	
Program about to run out of time	FINISH

XI DISPLAY AND ANALYSIS

Concentration values predicted by the Airshed Simulation Program are saved on binary files and are thus available for any display and analysis techniques that might be developed. At present, there is one program available to handle the airshed simulation output files. Currently, it can be used only for the display of the concentration data, but analysis capabilities can be easily added. In this chapter, the general capabilities of the display program are discussed, followed by descriptions and examples of its input and output. A detailed description of the program is given in the Systems Manual.

A. CAPABILITIES OF THE DISPLAY PROGRAM

The display program provides for two distinct operaing modes: prediction and comparison. In the "prediction" mode, concentration predictions are read from one airshed simulation run, and concentration maps and vertical concentration profiles are printed. Capabilities that could be added to the program in this mode include contour mapping of concentration isopleths and calculation of some simple statistics, such as hourly maximum concentrations for each species, frequency of exceeding certain specified levels, and concentrations averaged over time periods longer than that used by the simulation.

In the "comparison" mode, which has been provided for but not yet implemented, one set of concentrations would be subtracted from another, and all further display and analysis would be performed on the resulting array of differences. The comparison mode could be used for validating model predictions against observed data as well as assessing the impact of different model scenarios.

The display program is currently capable of processing a region of up to 30 x 30 grid cells in the horizontal plane, with a maximum of 13 chemical species. These maximum dimensions can be changed by recompiling the program.

B. INPUT REQUIRED BY THE DISPLAY PROGRAM

As illustrated in Figure XI-1, the input to the display program consists of the following:

> Card-supplied display options and print controls.
> Three data files used by the simulation program.
> One output concentration file from the simulation program.
> Optionally, a second concentration data file.

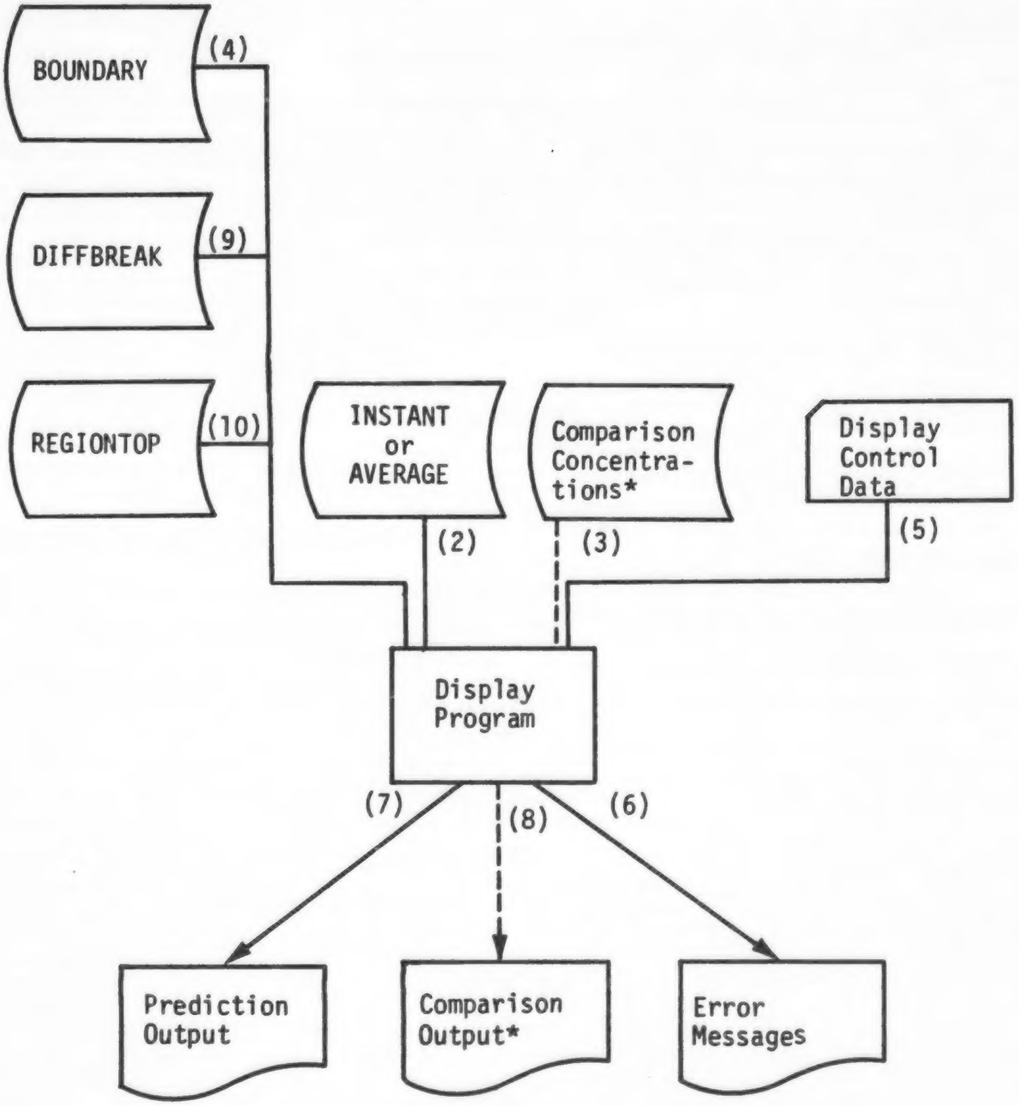
This section discusses first the data files that are to be input, and then details the contents and format of the input cards.

1. Data File Input

If concentration maps and vertical profiles are requested (currently the only features available), the BOUNDARY, DIFFBREAK, and REGIONTOP files used for the simulation run must be input. The BOUNDARY file describes the segmentation layout and defines the boundary of the simulated area in the horizontal plane. The DIFFBREAK and REGIONTOP files are used to calculate vertical heights at selected stations. If the simulation has been performed with more than 1 segment, it is the segmented versions of the BOUNDARY, DIFFBREAK, and REGIONTOP files that must be provided to the display program.

One of the Airshed Simulation Program output files containing predicted concentration values must also be input. The concentration values can be instantaneous (INSTANT) or averaged over a time interval (AVERAGE); the output intervals for both files are specified in the SIMCONTROL file. The display program recognizes the file type from the header record, and formats the output accordingly.

If a comparison run is to be made (an option not yet fully implemented), a second concentration file must also be input. This file could contain concentration fields gridded from observed data using the AIRQUALITY data preparation program, or it could contain the results from another airshed simulation run.


BOUNDARY
(4)
DIFFBREAK
(9)
REGIONTOP
(10)
INSTANT or AVERAGE
(2)
Comparison Concentrations*
(3)
Display Control Data
(5)
Display Program
(7)
(8)
(6)
Prediction Output
Comparison Output*
Error Messages

* This option is not yet available.

Figure XI-1. Information Flow Diagram for the Display Program

All input files must contain the same segment structure; that is, all must be either unsegmented or segmented according to the same segment layout.

2. Card Input

The display program requires the following data to be input on cards:

- Output display options
- Names of species to be examined
- Vertical level to be considered
- Print controls
- Measurement station and landmark names and locations
- Display units conversion factors
- User comments to appear on output.

The exact structure of each data card is shown in Table XI-1; Exhibit XI-1 is a sample input deck. Consistent with assumptions used in both the data preparation and simulation programs, the following conventions are generally followed in specifying data fields on each card:

- Integer input is in 10-character fields, up to six per card.
- Real number input is floating point in 10-character fields, up to six per card.
- Alphanumeric input is read and stored as one character per machine word.

Table XI-1. Display Program Control Input Definition

Card Number and Name	Item and Columns	Format	Comments
1 Output Options			
	KMAP 1-10	I10	Map selection flag: 1, if concentration maps are desired; 0, if no maps are desired
	KCOMP 11-20	I10	Comparison option selection flag: 1, if comparison of two concentration files is required; 0, if no comparison is required
	KSTNFL 21-30	I10	If greater than 0, writes station predictions to unit 12.
	KALLFL 31-40	I10	If greater than 0, writes concentration field predictions to unit 16.
2 Species Count	NSPECP 1-10	I10	Number of species to be examined: must be ≤ 13
3+ Species Names	((SPNAME(I,J), J = 1, 10), I = 1, NSPECP) 1-60	6(10A1)	Alphanumeric names of species to be examined--10 characters per name, left adjusted, six names per card; each name must correspond to a name used in the Airshed Simulation Program run; the species can be named in any order
4 Vertical Level	NLEVEL 1-10	I10	Vertical level to be examined and mapped
5 Map Print Times (only if KMAP = 1)			Print types must correspond to times for which data on the concentration data files are available
	DATPRS 1-10	I10	Print start date (Julian date)
	TPRS 11-20	F10.2	Print start time (hours past midnight)

Table XI-1 (Continued)

Card Number and Name	Item and Columns	Format	Comments
5 Map Print Times (con't)			
	DTPR 21-30	F10.2	Print interval (hours)
	DATPRF 31-40	I10	Print finish date (Julian date)
	TPRF 41-50	F10.2	Print finish time (hours past midnight)
The next four cards (Nos. 6 through 9) are to be input only for the comparison mode (not yet implemented)			
6 Comparison Times (only if KCOMP = 1)			Comparison times must correspond to times for which data on the data files are available
	DATSCS 1-10	I10	Comparison start date (Julian date)
	TSCS 11-20	F10.2	Comparison start time (hours past midnight)
	DTSC 21-30	F10.2	Comparison interval (hours)
	DATSCF 31-40	I10	Comparison finish date (Julian date)
	TSCF 41-50	F10.2	Comparison finish time (hours)
7 Comparison Station Count (only if KCOMP = 1)	NSTATC 1-10	I10	Number of stations at which concentrations are to be compared; must be ≤ 16; this number is used to determine how many Card 8's are to be read

Table XI-1 (Continued)

Card Number and Name	Item and Columns	Format	Comments
8+ Comparison Stations (only if KCOMP = 1)	((STATNA(I,J), J = 1, 20), I = 1, NSTATC) 1-60	3(20A1)	Alphanumeric names of stations at which concentrations are to be compared--20 characters per name, left adjusted, three names per card; each name must match a station name listed on Card 11.
9 Comparison Options (only if KCOMP = 1)			
	KPLOT 1-10	I10	Comparison plot flag: 1, if plots are desired; 0, if no plots are needed
	KSTAT 11-20	I10	Statistics option flag: 1, if comparative statistics are to be calculated; 0, if no statistics are to be calculated
10 Point Counts			
	NOSTN 1-10	I10	Number of stations at which concentrations are to be calculated--must be ≤ 16; stations are also included on concentration maps
	NOLAND 11-20	I10	Number of landmarks to be included on concentration maps--must be ≤ 8

Table XI-1 (Continued)

Card Number and Name	Item and Columns	Format	Comments
11+ Station			There must be NOSTN of these cards
	Station Name 1-20	20A1	Alphanumeric station name, left adjusted
	x-location 21-30	F10.0	x-coordinate of the station, measured in meters from the reference origin
	y-location 31-40	F10.0	y-coordinate of the station, measured in meters from the reference origin
12+ Landmark			There must be NOLAND of these cards
	Landmark name 1-20	20A1	Alphanumeric landmark name, left adjusted
	x-location 21-30	F10.0	x-coordinate of the landmark, measured in meters from the reference origin
	y-location 31-40	F10.0	y-coordinate of the landmark, measured in meters from the reference origin
13+ Output Units	(IOUNTS(I), I = 1, NSPECP) 1-60	6I10	Output conversion flags, six per card; the number and order must correspond to the species named on Cards 3+; internal units are in $\mu g/m^3$ for AEROSOLS and ppm for all other species; different units, however, can be selected for display output using IOUNTS as follows: 1 = ppm; 2 = pptm; 3 = pphm; 4 = ppb; 5 = $\mu g/m^3$

Table XI-1 (Concluded)

Card Number and Name	Item and Columns	Format	Comments
14 User Comment	NOTE 1-80	20A4	Note--up to 80 characters--written on header page of display output; it is referred to on that page as "*COMMENTS*"
15 Region Name	REGION 1-80	20A4	Region description note--up to 80 characters--to be used in entitling display output header page

```
         1         0
         9
NO        NO2       O3        ETH       OLE       PAR
CARB      ARO       CO
         1
     76195     05.00      1.00     76195     09.01
        21         0
101                    19183.0   27862.0
102                    17518.0   34045.0
103                    22588.0   30467.0
104                    22312.0   25304.0
105                    18706.0   24453.0
106                    13660.0   25566.0
107                    15179.0   30610.0
108                    23407.0   39102.0
109                    30802.0   27886.0
110                    22209.0   20826.0
111                    13812.0   20479.0
112                     8938.0   28913.0
113                    12738.0   37820.0
114                    19320.0   45456.0
115                    32111.0   45799.0
116                    37777.0   38083.0
117                    35560.0   20818.0
118                    18065.0   11256.0
119                     4759.0   18547.0
120                    -1921.0   33909.0
121                     7414.0   50376.0
         4         4         4         4         4         3
         4         4         2
                                  USER COMMENT
                                ST. LOUIS REGION
```

Exhibit XI-1. Sample Input for the Display Program

C. OUTPUT PRODUCED BY THE DISPLAY PROGRAM

The display program first prints a header page, including the alphanumeric region description supplied in the input deck, the dimensions of the simulated area of the grid, the input user comment, and the run identifier from the simulation run that produced the concentration predictions. A sample of the display program header page is shown in Exhibit XI-2.

The display program, operating in prediction mode, currently produces two types of output for each time interval on the input concentration file.

> Vertical concentration profiles. At each station location input, the concentrations at each vertical level are printed for each designated species. The heights of the diffusion break (mixing depth) and top of the region are also printed at each station. An example of vertical profile output is shown in Exhibit XI-3.

> Ambient concentration maps. Maps are printed of concentrations in all horizontal grid cells (excluding boundary cells) at the vertical level designated by the user. Printout is confined to those hours and species designated by the user. A separate map is produced for each species at each print time. Station sites and landmarks are also printed on each concentration map. An example of the concentration maps is shown in Exhibit XI-4.

Operating in comparison mode, the display program would calculate residuals for a designated vertical level by subtracting the concentration field on the "comparison" file from the corresponding field on the primary concentration file. Among the statistics calculated for these residuals would be the average value, standard deviation, and correlation coefficient. Calculation of other statistics could be readily incorporated into the program. These statistics would be calculated for each designated species at each print time. Maps of residuals could also be generated for each desired species at each specified print time.

```
                    URBAN SCALE AIR POLLUTION SIMULATION MODEL OF

                                 ST. LOUIS REGION

                                'INPUT PARAMETERS'

MESH SPACING IN X-DIRECTION   4.0000000+003          MESH SPACING IN Y-DIRECTION   4.0000000+003

NUMBER OF MESH POINTS IN X-DIRECTION , 15            NUMBER OF MESH POINTS IN Y-DIRECTION , 20

                          NUMBER OF VERTICAL MESH POINTS  4


                                    'COMMENTS'

                                   USER COMMENT

                                     'RUN ID'

                RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79
```

Exhibit XI-2. Standard Display Program Header Page

```
RUN ID =RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79

        VERTICAL AVERAGE CONCENTRATION PROFILES ABOVE SELECTED SITES ON  76195 BETWEEN THE HOURS OF    5. AND    6. LST

                  121                           MIXING DEPTH=  164.0 METERS,     TOP OF REGION=  564.0 METERS
NO       (PPB )        1.07          .61           .04          .06
NO2      (PPB )        8.87         8.26          2.32         2.63
O3       (PPB )       15.20        22.18         77.32        77.13
ETH      (PPB )        2.43         1.90          1.08         1.08
OLE      (PPB )        4.10         3.48          2.07         2.07
PAR      (PPHM)        7.57         5.90          3.32         3.32
CARB     (PPB )        7.15         6.45          4.29         4.29
ARO      (PPB )        2.64         2.12          1.22         1.22
CO       (PPTM)        1.61         1.27          1.02         1.00

                  115                           MIXING DEPTH=  201.4 METERS,     TOP OF REGION=  601.4 METERS
NO       (PPB )         .39          .17           .06          .06
NO2      (PPB )        5.15         4.17          2.89         2.88
O3       (PPB )       28.81        40.40         76.95        76.97
ETH      (PPB )        1.53         1.29          1.08         1.08
OLE      (PPB )        2.78         2.42          2.08         2.08
PAR      (PPHM)        4.84         4.00          3.32         3.32
CARB     (PPB )        4.98         4.67          4.28         4.27
ARO      (PPB )        1.65         1.44          1.22         1.22
CO       (PPTM)        1.27         1.17          1.01         1.00

                  114                           MIXING DEPTH=  235.9 METERS,     TOP OF REGION=  635.9 METERS
NO       (PPB )         .67          .33           .05          .06
NO2      (PPB )        8.88         7.04          2.48         2.83
O3       (PPB )       27.19        33.67         77.29        76.99
ETH      (PPB )        1.70         1.45          1.07         1.08
OLE      (PPB )        3.14         2.78          2.06         2.07
PAR      (PPHM)        5.59         4.58          3.28         3.32
CARB     (PPB )        5.69         5.30          4.30         4.29
ARO      (PPB )        1.94         1.65          1.22         1.22
CO       (PPTM)        1.18         1.04           .86         1.00

                  108                           MIXING DEPTH=  270.2 METERS,     TOP OF REGION=  670.2 METERS
NO       (PPB )         .83          .32           .06          .07
NO2      (PPB )       10.63         7.61          2.91         3.04
O3       (PPB )       26.26        37.10         76.93        76.83
ETH      (PPB )        2.01         1.51          1.08         1.08
OLE      (PPB )        3.35         2.79          2.06         2.07
PAR      (PPHM)        6.97         4.82          3.32         3.32
CARB     (PPB )        5.89         5.30          4.30         4.29
ARO      (PPB )        2.67         1.75          1.22         1.22
CO       (PPTM)        1.47         1.22          1.00         1.00

                  116                           MIXING DEPTH=  194.6 METERS,     TOP OF REGION=  594.6 METERS
NO       (PPB )         .54          .18           .06          .06
NO2      (PPB )        5.89         4.10          2.89         2.88
O3       (PPB )       30.56        44.22         77.00        76.98
```

Exhibit XI-3. Sample Vertical Concentration Profile Output--Prediction Mode

```
RUN ID =RAPS 4-KM DAY 195 -- 4-HR RUN 07/13/76   C-BOND II 8-79

PANEL 1          AVERAGE AMBIENT CONCENTRATIONS(PPB ) OF O3          ON  76195 BETWEEN THE HOURS OF    5. AND    6. LST

          2    3    4    5    6    7    8    9   10   11   12   13   14   15   16
     *                                                                               *
  21 *   22   21   21   21   21   21   22   22   23   24   24   24   23   23   21    * 21
     *                                                                               *
  20 *   20   19   18   18   18   19   20   21   23   24   24   24   23   24   23    * 20
     *                                                                               *
  19 *   18   17   16   15   16   18   20   20   20   22   24   24   23   24   23    * 19
     *                                                                               *
  18 *   17   15   13   13   14   16   20   21   20   19   20   24   25   25   24    * 18
     *                             121                                               *
  17 *   15   13   11   11   12   14   21   25   26   24   22   23   27   25   24    * 17
     *                                                                               *
  16 *   13   10    7    8   13   14   19   25   28   27   27   29   29   27   24    * 16
     *                                            114             115                *
  15 *   13   10    9   10   12   14   17   20   24   26   28   30   31   28   24    * 15
     *                                                 108                116        *
  14 *   15   14   12   12   15   18   19   20   24   26   30   32   32   30   25    * 14
     *                                     113   102                                 *
  13 *   10   13   12   13   17   18   17   16   21   26   33   33   32   30   26    * 13
     *                  120                  107       103                           *
  12 *    6   11   12   12   16   14   14   14   18   29   34   34   32   30   26    * 12
     *                                112         101            109                 *
  11 *   11    9   10   13   14   12    9    9   21   30   37   36   34   30   26    * 11
     *                                      106   105104                             *
  10 *   15   12   13   15   17   16   18   21   25   29   37   35   34   29   25    * 10
     *                           119        111       110              117           *
   9 *   17   15   13   14   17   18   19   22   31   33   33   32   31   28   25    *  9
     *                                                                               *
   8 *   18   17   15   15   14   16   22   26   29   31   32   31   29   27   25    *  8
     *                                           118                                 *
   7 *   18   17   17   17   17   19   21   26   28   30   31   31   29   26   24    *  7
     *                                                                               *
   6 *   19   18   18   18   18   22   24   25   27   29   31   31   29   23   23    *  6
     *                                                                               *
   5 *   20   20   19   19   18   22   24   25   27   28   28   27   26   24   23    *  5
     *                                                                               *
   4 *   22   21   20   19   18   23   24   25   26   26   27   27   26   24   23    *  4
     *                                                                               *
   3 *   23   22   21   19   15   25   25   25   26   26   26   26   25   24   23    *  3
     *                                                                               *
   2 *   23   23   23   22   22   24   24   25   25   25   25   25   25   24   23    *  2
```

Exhibit XI-4.   Sample Ambient Concentration Maps--Prediction Mode

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